Non-perturbative Improvement and Renormalization of the Axial Current

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Lattice Fields

Spinor Fields $\psi^{(f)}_{\mu,c}(x)$

- living on lattice sites

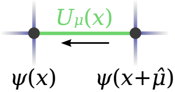
Gauge Fields $U_{\mu,c,c'}(x) \in \mathrm{SU}(3)$

- living on lattice links
- "integrated" version of $A_\mu(x) \in \mathfrak{su}(3)$

Gauge-Invariant Products

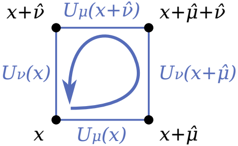
- lines

$$\bar{\psi}(x) \cdot U_\mu(x) \cdot \psi(x+\hat{\mu})$$



- loops

$$\mathrm{Tr}(P_{\mu\nu}(x)) = \mathrm{Tr}\big[U_\mu(x) \cdot U_\nu(x+\hat{\nu}) \cdot \\ \cdot U_\mu(x+\hat{\mu}+\hat{\nu})^{-1} \cdot U_\nu(x+\hat{\nu})^{-1}\big]$$

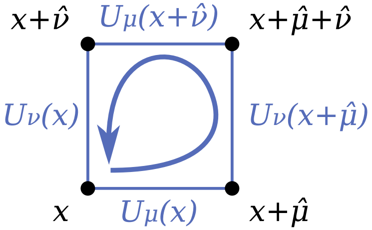


Gauge Action

Plaquette Action

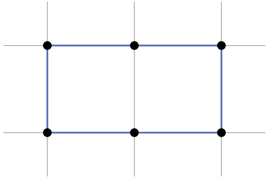
$$S_{\mathrm{Pl}}[U] = \frac{1}{g_0^2} \sum_{x,\mu\neq\nu} \mathrm{Tr}\left(1 - P_{\mu\nu}(x)\right)$$

- fundamental gauge action
- sum over traces of all 1×1 loops
- $\mathcal{O}(a^2)$ discretization errors



Tree-Level-Improved Lüscher–Weisz Action

- also 2×1 loops



Fermion Action

Wilson Action

$$S_{\mathrm{F}}[U,\psi,\bar{\psi}] = \sum_x \bar{\psi}(x)\left[\gamma_\mu \cdot \frac{1}{2}(\nabla_\mu + \nabla^*_\mu) + m - \underbrace{\frac{1}{2}\nabla^*_\mu\nabla_\mu}_{\text{Wilson term}}\right]\psi(x)$$

- ∇_μ, ∇^*_μ: forward and backward differences
- Wilson term removes "doublers"

Symanzik Improvement

- $\mathcal{O}(a)$ errors, because Wilson term breaks chiral symmetry
- improved to $\mathcal{O}(a^2)$ by
  - adding *clover term* to action — Bulava, Schaefer: arxiv:1304.7093
  - adding additional operators to quark bilinears (like axial current)

The Axial Current

Bare Axial Current

$$A_\mu(x) = \bar{\psi}(x)\,\gamma_\mu\gamma_5\,\psi(x)$$

- pseudovector
- flavor structure omitted

Example (Applications)

- PCAC quark masses (e.g. in tuning simulations)
- pseudoscalar decay constants (e.g. f_K, f_D, f_B)

A_μ must be...

- improved to remove $\mathcal{O}(a)$ lattice artifacts
- renormalized due to broken chiral symmetry
- ideally in a non-perturbative way

Outline

Symanzik Improvement Programm

- describe lattice action and fields by effective continuum theory

$$\phi_{\text{lat}}(x) = \phi_{\text{con}}(x) + a^1\phi_1(x) + a^2\phi_2(x) + a^3\phi_3(x) + \dots$$

- $\phi_n(x)$ is linear combination of all local operators with correct dimension and symmetries
- subtract $\mathcal{O}(a)$ terms

Symanzik Improvement Programm

Example (Derivative)

- let f be a real function, $f : \mathbb{R} \to \mathbb{R}$
- symmetric difference $\tilde{\nabla}_a f(x) := [f(x+a) - f(x-a)]/(2a)$
- can be expressed using Taylor series

$$\tilde{\nabla}_a f(x) = f'(x) + a^2 \cdot \frac{f^{(3)}(x)}{6} + a^4 \cdot \frac{f^{(5)}(x)}{120} + \mathcal{O}(a^6)$$

- due to symmetry, only odd derivatives contribute
- subtract discretized version of a^2 term

$$\tilde{\nabla}_a f(x) - \frac{a^2}{6} \tilde{\nabla}_a^3 f(x) = f'(x) + \mathcal{O}(a^3)$$

Improvement of Axial Current

$$A_\mu(x) = \bar{\psi}(x)\,\gamma_\mu\gamma_5\,\psi(x)$$

- A_μ is pseudovector with mass dimension 3
  $\mathcal{O}(a)$ terms must have dimension 4
- possible operators at $\mathcal{O}(a)$:

$$O_1 = \bar{\psi}\gamma_5\sigma_{\mu\nu}D_\nu\psi - \bar{\psi}\overleftarrow{D}_\nu\sigma_{\mu\nu}\gamma_5\psi$$

$$O_2 = \partial_\mu\left(\bar{\psi}\gamma_5\psi\right) \qquad O_3 = m\bar{\psi}\gamma_\mu\gamma_5\psi$$

- on shell, O_1 and O_3 connected through e.o.m. $\Rightarrow$ drop O_1
- O_3 regarded as mass-dependent renormalization (see later)
- improved axial current:

$$(A_\mathrm{I})_\mu(x) = A_\mu(x) + a c_\mathrm{A} \cdot \tilde{\partial}_\mu P(x)$$

Determination of c_A

Partial Conservation of Axial Current (PCAC)

$$\langle \partial_\mu A_\mu(x) \cdot X \rangle = 2m \cdot \langle P(x) \cdot X \rangle$$

- continuum Ward identity, valid for any external operator X
- used to define PCAC quark mass
- broken by $\mathcal{O}(a)$ terms on lattice

Idea

- choose two different external operators X
- for each, compute PCAC mass using improved A_μ
- adjust c_A so that both are equal

Determination of c_A

$$\frac{\langle \partial_\mu A_\mu X_1 \rangle + a c_A \langle \partial_\mu^2 P X_1 \rangle}{2 \langle P X_1 \rangle} \stackrel{!}{=} m \stackrel{!}{=} \frac{\langle \partial_\mu A_\mu X_2 \rangle + a c_A \langle \partial_\mu^2 P X_2 \rangle}{2 \langle P X_2 \rangle}$$

- solved for c_A:

$$c_A = -\frac{1}{a} \cdot \frac{r_1(x) - r_2(x)}{s_1(x) - s_2(x)}$$

with

$$r_i(x) = \frac{\left\langle \tilde{\partial}_\mu A_\mu(x) X_i \right\rangle}{2 \langle P(x) X_i \rangle} \qquad s_i(x) = \frac{\langle \partial_\mu^2 P(x) X_i \rangle}{2 \langle P(x) X_i \rangle}$$

What operators X_1 and X_2 should we choose?

Previous Works in the Alpha Collaboration

$N_f = 0$ (hep-lat/9609035)

- Schrödinger functional
- $X_1 = X_2$, but different periodicity angle θ
  $\rightarrow$ low sensitivity for $L \gtrsim 0.8\,\mathrm{fm}$
  $\rightarrow$ $N_\mathrm{f} > 0$ would require individual simulations

$N_f = 2$ (hep-lat/0503003)

$N_f = 3$ and Iwasaki gauge action (hep-lat/0703006)

- Schrödinger functional
- X_1 and X_2 pseudoscalars with different wave functions $\omega_{\pi^{(0)}}, \omega_{\pi^{(1)}}$, sensitivity $\propto m^2_{\pi^{(1)}} - m^2_{\pi^{(0)}}$

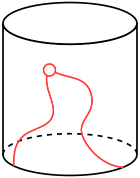
Schrödinger Functional

- periodic BC in space, Dirichlet in time
- pseudoscalar source operator at $t = 0$ boundary

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

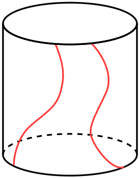
(boundary fields $\zeta(\mathbf{x}) \propto \psi(a, \mathbf{x})$)

- correlators that we need:



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

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



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

Wave Functions

Idea

choose WF $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$ that couple only to the ground and first excited state

- define basis functions

$$\omega_1(r) = \mathrm{e}^{-r/r_0} \qquad \omega_2(r) = r \cdot \mathrm{e}^{-r/r_0} \qquad \omega_3 = \mathrm{e}^{-r/(2r_0)}$$

- make them periodic to fit BC
- compute 3×3 matrix $F_1(\omega_i, \omega_j)$
- determine eigenvalues $\lambda^{(0)} > \lambda^{(1)} > \lambda^{(2)}$ and eigenvectors $\eta^{(0)}$, $\eta^{(1)}$, $\eta^{(2)}$
- approximate $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$ by

$$\omega_{\pi^{(0)}} \approx \sum_i \eta_i^{(0)} \omega_i \qquad \omega_{\pi^{(1)}} \approx \sum_i \eta_i^{(1)} \omega_i$$

Final Improvement Condition

$$c_\mathrm{A} = -\frac{1}{a} \cdot \frac{r_1(x_0) - r_2(x_0)}{s_1(x_0) - s_2(x_0)}$$

with

$$r_i(x_0) = \frac{\tilde{\partial}_0 f_A(x_0; \omega_{\pi(i)})}{2 \cdot f_P(x_0; \omega_{\pi(i)})} \qquad s_i(x_0) = \frac{\partial_\mu^2 f_P(x_0; \omega_{\pi(i)})}{2 \cdot f_P(x_0; \omega_{\pi(i)})}$$

- we have chosen $x_0 = L/2$

Renormalization of Axial Current

Improvement:	$(A_\mathrm{I})^a_\mu(x) = A^a_\mu(x) + ac_A \cdot \tilde{\partial}_\mu P^a(x)$	✓
Renormalization:	$(A_\mathrm{R})^a_\mu(x) = Z_\mathrm{A} \cdot (1 + b_\mathrm{A} am_\mathrm{q}) \cdot (A_\mathrm{I})^a_\mu(x)$	2do

- leading coefficient $\rightarrow$ sensitive to errors

same basic strategy as before:

- find suitable continuum Ward identity
- choose Z_A so that it holds on lattice, too
- mass-dependent term $\propto b_\mathrm{A}$ will be ignored $(m_q \rightarrow 0)$

Renormalization Condition

- based on chiral Ward identity, similar to PCAC[1]
- in addition, a second axial current $A_0(y)$

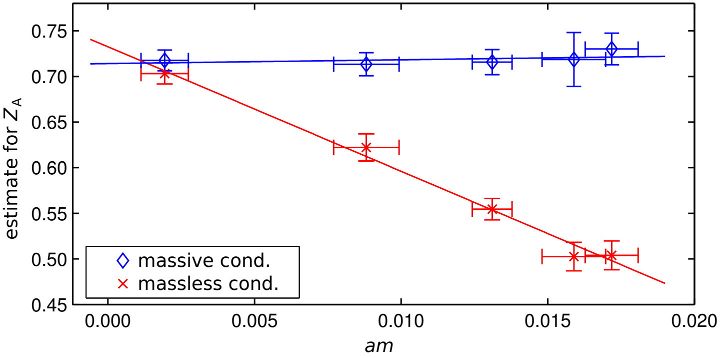
$$\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\,\epsilon^{abc}\left\langle A_0^a(x)\cdot A_0^b(y)\,O_{\mathrm{ext}}^c\right\rangle$$
$$-2m\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\,\epsilon^{abc}\int_{y_0}^{x_0}\mathrm{d}x_0'\left\langle P^a(x_0',\mathbf{x})\cdot A_0^b(y)\,O_{\mathrm{ext}}^c\right\rangle$$
$$=\mathrm{i}\int \mathrm{d}^3\mathbf{y}\,\langle V_0^c(y)\,O_{\mathrm{ext}}^c\rangle$$

- RHS due to variation of second A_0 insertion
- non-vanishing PCAC mass is explicitly taken into account to facilitate extrapolation to $m=0$

[1] $\partial_\mu A_\mu = 2mP$

Renormalization Condition

comparison of the chiral extrapolation at $\beta = 5.2$, taken from $N_\mathrm{f} = 2$:



arxiv:hep-lat/0505026, fig. 2

Correlators

$$\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\,\epsilon^{abc}\left\langle A_0^a(x)\,A_0^b(y)\,O_{\mathrm{ext}}^c\right\rangle$$

$$-2m\int \mathrm{d}^3\mathbf{x}\mathrm{d}^3\mathbf{y}\,\epsilon^{abc}\int_{y_0}^{x_0}\mathrm{d}x_0'\left\langle P^a(x_0',\mathbf{x})\,A_0^b(y)\,O_{\mathrm{ext}}^c\right\rangle$$

$$= \mathrm{i}\int \mathrm{d}^3\mathbf{y}\,\langle V_0^c(y)\,O_{\mathrm{ext}}^c\rangle$$

- $O_{\mathrm{ext}}^c \propto \epsilon^{cde} O'^d(\omega_{\pi(0)}) O^e(\omega_{\pi(0)})$ as source and sink operator
- in terms of renormalized Schrödinger-functional correlators:

$$Z_{\mathrm{A}}^2 \cdot \left[F_{\mathrm{AA}}^{\mathrm{I}}(x_0,y_0) - 2m\cdot\tilde{F}_{\mathrm{PA}}^{\mathrm{I}}(x_0,y_0)\right] = F_1$$

Renormalization Condition

$$Z_{\mathrm{A}}(g_0^2) = \lim_{m\to 0}\sqrt{F_1}\left[F_{\mathrm{AA}}^{\mathrm{I}}(x_0,y_0) - 2m\cdot\tilde{F}_{\mathrm{PA}}^{\mathrm{I}}(x_0,y_0)\right]^{-1/2}$$

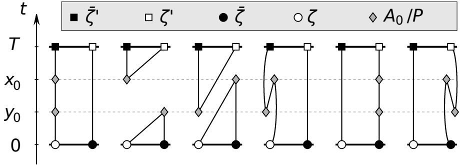
Correlators

$$F_{XY}(x_0, y_0) = -\frac{a^6}{6L^6} \sum_{\mathbf{x},\mathbf{y}} \varepsilon^{abc} \varepsilon^{cde} \left\langle O'^d \cdot X^a \cdot Y^b \cdot O^e \right\rangle$$

with insertions of

$$A_0^a(x_0), \qquad \partial_0 P^a(x_0), \qquad \tilde{P}^a(x, y_0) = \sum_{t=y_0}^{x_0} w(t) \cdot P^a(t, \mathbf{x})$$

Connected and Disconnected Contributions:



- standard choice: $x_0 = 2/3 \cdot T$ and $y_0 = 1/3 \cdot T$
- implemented in SFCF code and checked against old results
- alternative definition $Z_{\mathrm{A,con}}$ with connected only

Evaluating Expectation Values on the Lattice

$$\left\langle O(U,\psi,\bar{\psi})\right\rangle = \frac{1}{Z}\int [\mathrm{d}U][\mathrm{d}\psi][\mathrm{d}\bar{\psi}]\, O(U,\psi,\bar{\psi})\,\mathrm{e}^{-S_{\mathrm{G}}(U)-S_{\mathrm{F}}(U,\psi,\bar{\psi})}$$

1. generate gauge-field configurations with probability $\propto$ Boltzmann factor
2. for each config, evaluate fermionic integral to compute f_{A}, $f_{\mathrm{P}}, \ldots$ ("primary observables")
3. average over all gauge configs
4. analysis: compute c_{A} and Z_{A}

General Remarks

- generation of gauge configurations by openQCD code with Schrödinger-functional BC

  Lüscher, Schaefer (arxiv:1206.2809)

  - frequency splitting of the quark determinant
  - Zolotarev rational approximation for third quark $\rightarrow$ reweighting
  - two- and three-level integration schemes
- Schrödinger-functional setup
  - $\theta = 0$, vanishing background field
  - $T = 3/2 \cdot L$ with $L \approx 1.2\,\mathrm{fm}$

Line of Constant Physics

- keep physical scales fixed through all simulations
  $\Rightarrow$ $\mathcal{O}(a)$ cutoff effects vanish smoothly
  $\Rightarrow$ prevent large $\mathcal{O}(a)$ ambiguities in c_A itself
- coupling $\beta = 6/g_0^2$ tuned to keep $L \approx 1.2\mathrm{fm}$ constant through all lattice sizes via perturbative formula ($g_0 < g_0'$)

$$\frac{a(g_0^2)}{a(g_0'^2)} = \mathrm{e}^{-\left(g_0^{-2} - g_0'^{-2}\right)/(2b_0)} \left(g_0^2/g_0'^2\right)^{-b_1/(2b_0^2)} \times \left[1 + q\left(g_0^2 - g_0'^2\right) + \mathcal{O}(g_0'^4)\right]$$

- κ tuned to get almost vanishing (PCAC) quark mass

Parameters

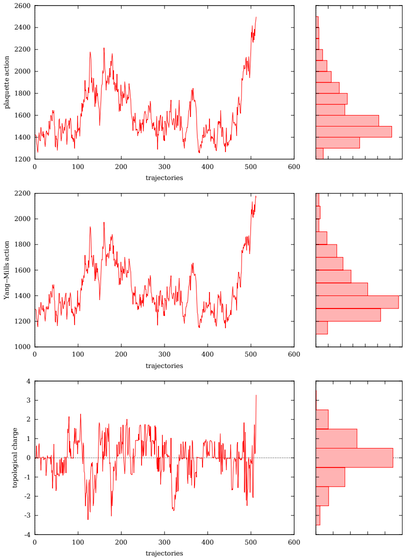
L/a	T/a	β	κ	N_{tr}	am_{PCAC}	$\bar{g}^2_{\mathrm{GF}}(L)$
12	17	3.300	0.13652	5120	−0.00096(71)	18.12(21)
12	17	3.300	0.13660	6524	−0.0086(6)	16.92(13)
16	23	3.512	0.13700	10240	0.0064(2)	16.49(13)
16	23	3.512	0.13703	4096	0.0056(3)	16.85(20)
16	23	3.512	0.13710	12288	0.0024(2)	16.11(14)
20	29	3.676	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)

- trajectory length of 2 MDU
- acceptance $\gtrsim 0.90$
- check LCP by gradient flow coupling

Example Histories ($L/a = 12$)

plaquette action, Yang–Mills action and topological charge Q for

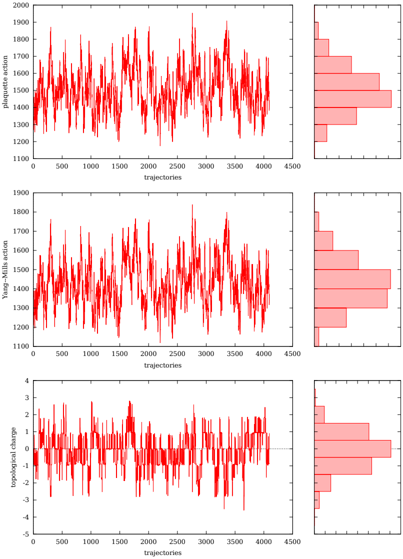
- $L/a = 12,\ T/a = 17$
- $\beta = 3.300$
- $\kappa = 0.13652$
- $N_{\text{tr}} = 512$



Example Histories ($L/a = 16$)

plaquette action, Yang–Mills action and topological charge Q for

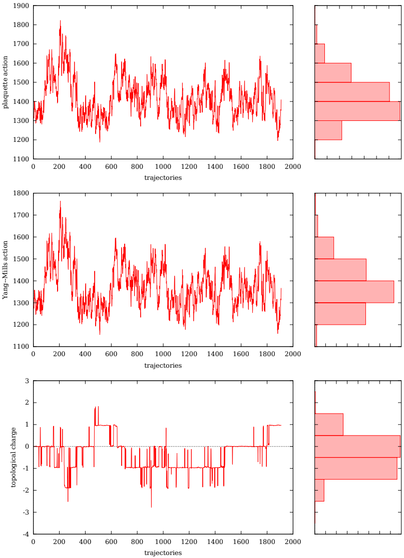
- $L/a = 16,\ T/a = 23$
- $\beta = 3.512$
- $\kappa = 0.13703$
- $N_{\mathrm{tr}} = 4096$



Example Histories ($L/a = 20$)

plaquette action, Yang–Mills action and topological charge Q for

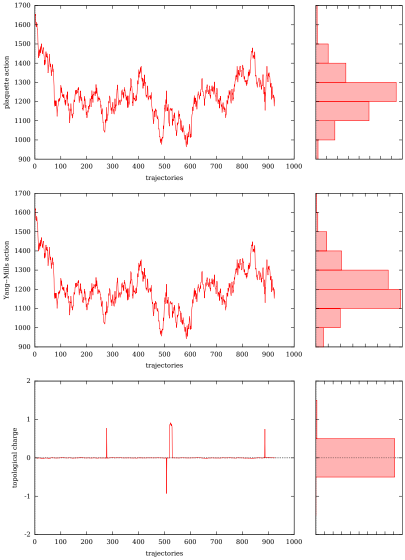
- $L/a = 20,\ T/a = 29$
- $\beta = 3.676$
- $\kappa = 0.13700$
- $N_{\mathrm{tr}} \approx 2000$



Example Histories ($L/a = 24$)

plaquette action, Yang–Mills action and topological charge Q for

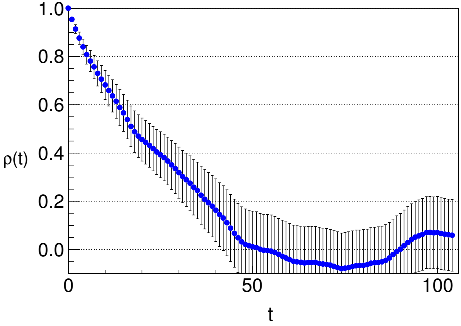
- $L/a = 24, \; T/a = 35$
- $\beta = 3.810$
- $\kappa = 0.13712$
- $N_{\text{tr}} \approx 900$

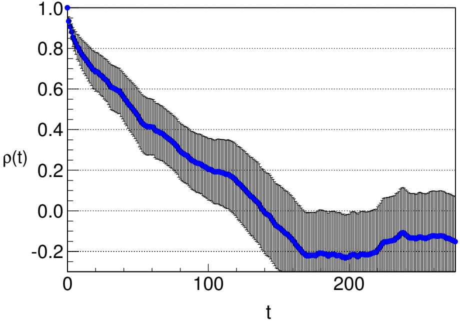


Analysis of Autocorrelations

Normalized autocorrelations functions at

$$L/a = 20, \qquad T/a = 29, \qquad \kappa = 0.1370$$

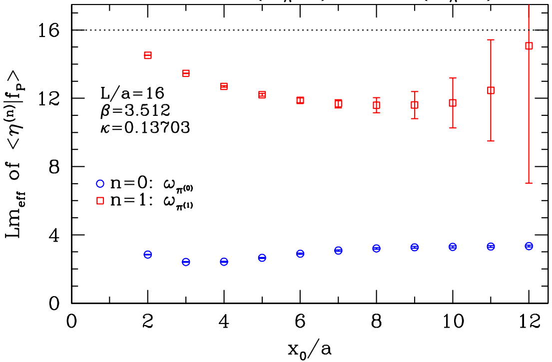




- Smoothed action: $\tau_{\text{int}} \approx 20 - 30$
- Topol. charge: $\tau_{\text{int}} \approx 60 - 70$

Effective Masses of $\omega_{\pi(0)}$ and $\omega_{\pi(1)}$ States

Energies of the states created by $O(\omega_{\pi(0)})$ and $O(\omega_{\pi(1)})$

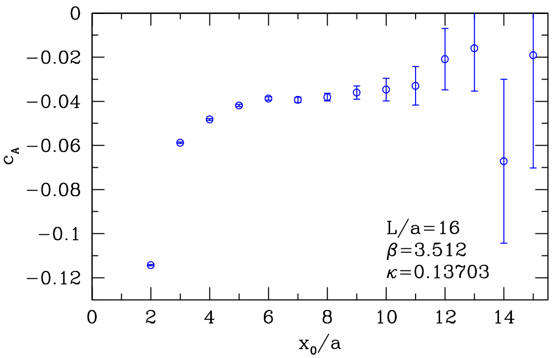


- clearly separated up to $x_0 \approx 12a \rightarrow$ good sensitivity for c_A
- first excited state still acceptably below the cutoff a^{-1}
  $\rightarrow$ probably significant $\mathcal{O}(a^2)$ effects in smaller volumes

Local $c_A(x_0)$

c_A measured at time coordinate x_0 and

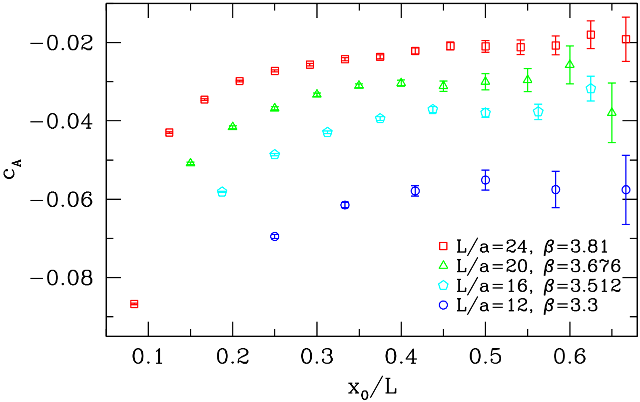
$$L/a = 16, \qquad \beta = 3.512, \qquad \kappa = 0.13703$$



- plateau starts at $x_0 \approx 5a$
- final definition at $x_0 = L/2$ (i.e. $x_0 = 8a$ for $L/a = 16$)

Local $c_A(x_0)$

local c_A from all simulations combined and appropriately scaled



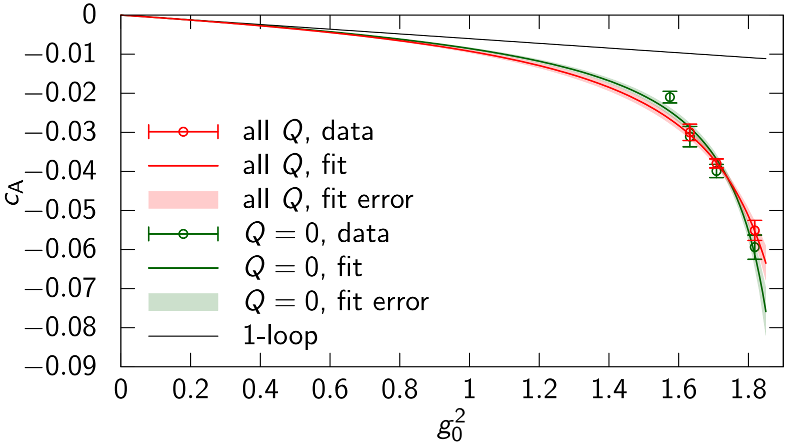
- $x_0 = L/2$ always lies well within the plateau
- acceptable signal-to-noise ratio

c_A Table

lattice	β	κ	$c_A(L/2)$	$c_A(L/2)\|_{Q=0}$
$12^3 \times 17$	3.300	0.13652	$-0.0551(26)$	$-0.0594(31)$
$12^3 \times 17$	3.300	0.13660	$-0.0557(19)$	–
$16^3 \times 23$	3.512	0.13700	$-0.0365(11)$	$-0.0348(15)$
$16^3 \times 23$	3.512	0.13703	$-0.0381(16)$	$-0.0334(29)$
$16^3 \times 23$	3.512	0.13710	$-0.0380(11)$	$-0.0399(17)$
$20^3 \times 29$	3.676	0.13680	$-0.0324(14)$	$-0.0305(29)$
$20^3 \times 29$	3.676	0.13700	$-0.0300(21)$	$-0.0311(26)$
$24^3 \times 35$	3.810	0.13712	$-0.0210(15)$	$-0.0210(15)$

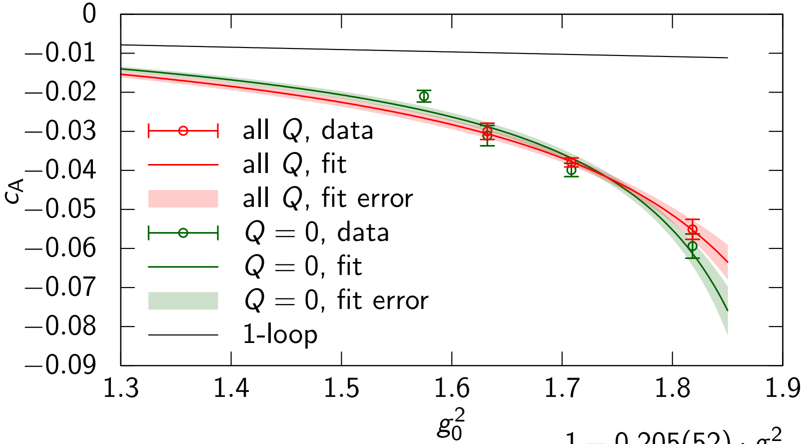
- c_A measured on $Q = 0$ configs is compatible

c_A versus Coupling



fit (all Q): $$c_A(g_0^2) \approx -0.006033 \cdot g_0^2 \cdot \frac{1 - 0.205(52) \cdot g_0^2}{1 - 0.48155(16) \cdot g_0^2}$$

c_A versus Coupling



fit (all Q): $$c_A(g_0^2) \approx -0.006033 \cdot g_0^2 \cdot \frac{1 - 0.205(52) \cdot g_0^2}{1 - 0.48155(16) \cdot g_0^2}$$

First Results

L/a	T/a	β	κ	N_{tr}	$Z_{A,con}$	Z_A
12	17	3.300	0.13652	5120	0.817(50)	0.655(50)
12	17	3.300	0.13660	6310	0.830(50)	0.649(50)
16	23	3.512	0.13700	5120	0.772(50)	0.764(50)
16	23	3.512	0.13703	–	–	–
16	23	3.512	0.13710	1648	0.800(50)	0.752(50)
20	29	3.676	0.13680	–	–	–
20	29	3.676	0.13700	7568	0.790(10)	0.790(20)
24	35	3.810	0.13712	–	–	–

- N_{tr} are the trajectories analyzed *so far*
- $Z_{A,con}$ not yet conclusive (need more statistics)
- Z_A: no strong mass dependence observed

Summary

Methods

- axial current is ingredient in many observables
- improvement and renormalization conditions based on chiral Ward identities that are restored at $\mathcal{O}(a)$ on the lattice
- evaluation in Schrödinger-functional setup
- external source operators with wave functions $\omega_{\pi^{(0)}}$ and $\omega_{\pi^{(1)}}$

Status of Results

- c_{A} to be published soon
- Z_{A}: many measurements to be done yet, crosscheck analysis
- maybe new simulations at smaller masses needed for Z_{A}

Outlook

- determination of Z_{V}

Thank you!