# Improved analysis of nucleon isovector charges and twist-2 matrix elements on CLS $N_f = 2+1$ ensembles

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in collaboration with

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# Observables

We want to compute nucleon forward matrix elements of **isovector** operator insertions $\mathcal{O}$

$$\left\langle N(p',s')\,|\mathcal{O}|\,N(p,s)\right\rangle .$$

- For **local** operators ($\to g_A,\ g_T,\ g_S$):

$$\mathcal{O}^A_\mu = \bar{q}\gamma_\mu\gamma_5 q, \quad \mathcal{O}^S = \bar{q}q, \quad \mathcal{O}^T_{\mu\nu} = \bar{q}i\sigma_{\mu\nu}q\,. \tag{1}$$

- For **one-derivative, dimension-four** operators ($\to \langle x\rangle_{u-d},\ \langle x\rangle_{\Delta u-\Delta d},\ \langle x\rangle_{\delta u-\delta d}$):

$$\mathcal{O}^{vD}_{\mu\nu} = \bar{q}\gamma_{\{\mu}\overleftrightarrow{D}_{\nu\}}\,q\,, \quad \mathcal{O}^{aD}_{\mu\nu} = \bar{q}\gamma_{\{\mu}\gamma_5\overleftrightarrow{D}_{\nu\}}\,q\,, \quad \mathcal{O}^{tD}_{\mu\nu\rho} = \bar{q}\sigma_{[\mu\{\nu]}\overleftrightarrow{D}_{\rho\}}\,q\,, \tag{2}$$

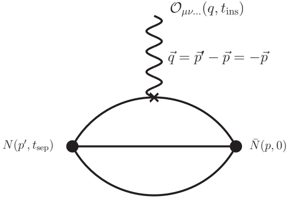
NMEs are obtained from the usual ratio with projectors $\Gamma_0 = \frac{1}{2}(1+\gamma_0)$ and $\Gamma_z = \Gamma_0(1+i\gamma_5\gamma_3)$

$$R^{\mathcal{O}}_{\mu_1,\ldots,\mu_n}(t_{\mathrm{sep}},t_{\mathrm{ins}}) \equiv \frac{C^{\mathcal{O},3\mathrm{pt}}_{\mu_1,\ldots\mu_n}(\vec{q}=0,t_{\mathrm{sep}},t_{\mathrm{ins}};\Gamma_z)}{C^{2\mathrm{pt}}(\vec{q}=0,t_{\mathrm{sep}};\Gamma_0)}\,. \tag{3}$$

- Extraction of ground state NMEs requires dedicated analysis for $t_{\mathrm{sep}} \lesssim 1.5\,\mathrm{fm}$.
- Final results for each observable from chiral, continuum and finite volume extrapolation.

# General Setup

- $N_f = 2+1$ flavors of non-perturbatively improved Wilson clover fermions. *JHEP 1502 (2015) 043*
- Lüscher-Weisz gauge action *Commun.Math.Phys. 97 (1985)*
- Exceptional configurations are suppressed by a twisted mass regulator. *PoS LATTICE2008 (2008) 049*
- Full non-perturbative renormalization (SF) available for $g_A$. Eur.Phys.J.C 79 (2019) 1, 23
- For other observables non-perturbative renormalization (RI'-MOM) at $\beta = 3.40, 3.46, 355$; Extrapolation for $\beta = 3.7$ as in 2019 paper. Phys.Rev.D 100 (2019) 3, 034513
- For 3pt functions we use sequential inversions through the sink, setting $p' = 0$.
- Only quark-connected 3pt functions contribute for isovector NMEs.
- Truncated solver method gives speedup of 2-5:
  *Comput.Phys.Commun. 181 (2010) 1570-1583*
  *Phys.Rev. D91 (2015) no.11, 114511*




$$\langle \mathcal{O} \rangle = \langle \frac{1}{N_{LP}} \sum_{i=1}^{N_{LP}} \mathcal{O}_n^{LP} \rangle + \langle \mathcal{O}_{\rm bias} \rangle , \quad \mathcal{O}_{\rm bias} = \frac{1}{N_{HP}} \sum_{i=1}^{N_{HP}} (\mathcal{O}_n^{HP} - \mathcal{O}_n^{LP}) .$$

Actual source setup depends on $t_{\rm sep}$ and boundary conditions ...

# Lattice setup (2019)

Phys.Rev.D 100 (2019) 3, 034513

| ID | $\beta$ | T/a | L/a | $M_\pi\,/\,\mathrm{GeV}$ | $M_\pi L$ | $N_{\mathrm{conf}}$ | $N_{\mathrm{meas}}$ | $t_{\mathrm{sep}}^{\mathrm{lo}}\,/\,\mathrm{fm}$ | $t_{\mathrm{sep}}^{\mathrm{hi}}\,/\,\mathrm{fm}$ | twist-2 |
|---|---|---|---|---|---|---|---|---|---|---|
| C101 | 3.40 | 96 | 48 | 0.223(3) | 4.68 | 2000 | 64000 | 1.04 | 1.38 | yes |
| H105 | 3.40 | 96 | 32 | 0.278(4) | 3.90 | 1019 | 48912 | 1.04 | 1.38 | yes |
| H102 | 3.40 | 96 | 32 | 0.352(4) | 4.93 | 1997 | 7988 | 1.04 | 1.38 | no |
| N401 | 3.46 | 128 | 48 | 0.287(4) | 5.33 | 701 | 11216 | 1.07 | 1.53 | yes |
| S400 | 3.46 | 128 | 32 | 0.350(4) | 4.34 | 1725 | 27600 | 1.07 | 1.53 | yes |
| D200 | 3.55 | 128 | 64 | 0.203(3) | 4.23 | 1021 | 32672 | 1.03 | 1.41 | yes |
| N200 | 3.55 | 128 | 48 | 0.283(3) | 4.42 | 1697 | 20364 | 1.03 | 1.41 | yes |
| S201 | 3.55 | 128 | 32 | 0.293(4) | 3.05 | 2092 | 66944 | 1.03 | 1.41 | yes |
| N203 | 3.55 | 128 | 48 | 0.347(4) | 5.42 | 1540 | 24640 | 1.03 | 1.41 | yes |
| J303 | 3.70 | 192 | 64 | 0.262(3) | 4.24 | 531 | 8496 | 1.00 | 1.40 | yes |
| N302 | 3.70 | 128 | 48 | 0.353(4) | 4.28 | 1177 | 18832 | 1.00 | 1.40 | yes |

- Only ensembles with open boundary conditions in time. *Comput. Phys. Commun. 184 (2013)*
- Only source-sink separations with $1.0\,\mathrm{fm} \lesssim t_{\mathrm{sep}} \lesssim 1.5\,\mathrm{fm}$.
- Fixed number of sources on a single timeslice; independent of $t_{\mathrm{sep}}$.
- Excited state treatment by simultanous two-state fit to the ratio in all six observables (where available) with a common gap $\Delta$ as free parameter:

$$R(t_{\mathrm{ins}}, t_{\mathrm{sep}}) = c_0 + c_1\left(e^{-\Delta t_{\mathrm{ins}}} - e^{-\Delta(t_{\mathrm{sep}} - t_{\mathrm{ins}})}\right) + c_2 e^{-\Delta t_{\mathrm{sep}}}$$

- Summation method only as cross-check; stat. larger errors due to small number of $t_{\mathrm{sep}}$'s.

# Lattice setup (2021)

| ID | $\beta$ | T/a | L/a | $M_\pi$ / GeV | $M_\pi L$ | $N_{\rm conf}$ | $N_{\rm meas}$ | $t^{\rm lo}_{\rm sep}$ / fm | $t^{\rm hi}_{\rm sep}$ / fm | twist-2 |
|---|---|---|---|---|---|---|---|---|---|---|
| C101 | 3.40 | 96 | 48 | 0.2250(12) | 4.73 | 2000 | 64000 | **0.35** | 1.38 | yes |
| H105 | 3.40 | 96 | 32 | 0.2805(27) | 3.93 | 1027 | 49296 | **0.35** | 1.38 | yes |
| H102 | 3.40 | 96 | 32 | 0.3544(11) | 4.96 | 2005 | 32080 | **0.35** | 1.38 | yes |
| D450 | 3.46 | 128 | 64 | 0.2162(07) | 5.35 | 500 | 64000 | **0.31** | 1.53 | yes |
| N451 | 3.46 | 128 | 48 | 0.2860(05) | 5.31 | 1011 | 129408 | **0.31** | 1.53 | yes |
| S400 | 3.46 | 128 | 32 | 0.3496(11) | 4.33 | **2873** | **45968** | **0.31** | 1.53 | yes |
| E250 | 3.55 | 192 | 96 | 0.1299(09) | 4.06 | 250 | 64000 | **0.26** | 1.41 | yes |
| D200 | 3.55 | 128 | 64 | 0.2024(07) | 4.22 | **2000** | **64000** | **0.26** | 1.41 | yes |
| N200 | 3.55 | 128 | 48 | 0.2811(09) | 4.39 | 1712 | 20544 | **0.26** | 1.41 | yes |
| S201 | 3.55 | 128 | 32 | 0.2924(16) | 3.05 | 2093 | 66976 | **0.26** | 1.41 | yes |
| N203 | 3.55 | 128 | 48 | 0.3449(08) | 5.41 | 1543 | 24688 | **0.26** | 1.41 | yes |
| J303 | 3.70 | 192 | 64 | 0.2596(08) | 4.19 | **1073** | **17168** | **0.20** | 1.40 | yes |
| N302 | 3.70 | 128 | 48 | 0.3485(08) | 4.22 | **2201** | **35216** | **0.20** | 1.40 | yes |

- **Added three new ensembles with peridioc BC; one (E250) with $M_\pi \approx M_\pi^{\rm phys}$.**
- **Additional source-sink separations available down to $t^{\rm lo}_{\rm sep} = 4a$ in steps of $\delta t_{\rm sep} = 2a$ on all ensembles.**
- **(Roughly) doubled statistics on several ensembles.**
- **Scaling of statistics:**
  - **$N_{\rm meas}$ reduced by factor of two at each or every second value of $t_{\rm sep} < 1\,{\rm fm}$.**
  - **pBC boxes: Sources are randomly distributed and statistics is doubled also at each value of $t_{\rm sep} > 1\,{\rm fm}$ (i.e. $N_{\rm meas}$ refers to $t^{\rm hi}_{\rm sep}$).**

# Two-state truncation for summation method

The two-state truncation of the summed ratio $S(t_{\rm sep}, t_{\rm ex}) = \sum_{t_{\rm ins}=t_{\rm ex}}^{t_{\rm sep}-t_{\rm ex}} R(t_{\rm ins}, t_{\rm sep})$ reads

$$
\begin{aligned}
S(t_{\rm sep}, t_{\rm ex}) =& M_{00}\left(1 - \frac{|A_1|^2}{|A_0|^2} e^{-\Delta t_{\rm sep}}\right)(t_{\rm sep} - 2t_{\rm ex} + 1) \\
&+ 2M_{01}\,\mathrm{Re}\left[\frac{A_1}{A_0}\right] \frac{e^{-\Delta t_{\rm ex}} - \left(e^{\Delta(t_{\rm ex}-1)} + \frac{|A_1|^2}{|A_0|^2} e^{-\Delta t_{\rm ex}}\right) e^{-\Delta t_{\rm sep}}}{1 - e^{-\Delta}} \\
&+ M_{11} \frac{|A_1|^2}{|A_0|^2} e^{-\Delta t_{\rm sep}} (t_{\rm sep} - 2t_{\rm ex} + 1) + \mathcal{O}(e^{-2\Delta t_{\rm sep}}),
\end{aligned} \tag{4}
$$

- $M_{ij}$ parameters denote matrix elements.
- $\Delta$ is the leading energy gap.
- $A_{0,1}$ are amplitudes of the two-point function.

Redefining $M_{01}$, $M_{11}$ to absorb ambiguous terms yields:

$$
\boxed{
\begin{aligned}
S(t_{\rm sep}, t_{\rm ex}) = & M_{00}(t_{\rm sep} - 2t_{\rm ex} + 1) + 2\tilde{M}_{01} \frac{e^{-\Delta t_{\rm ex}} - \left(e^{\Delta(t_{\rm ex}-1)} + \frac{|A_1|^2}{|A_0|^2} e^{-\Delta t_{\rm ex}}\right) e^{-\Delta t_{\rm sep}}}{1 - e^{-\Delta}} \\
& + \tilde{M}_{11} e^{-\Delta t_{\rm sep}} (t_{\rm sep} - 2t_{\rm ex} + 1) + \mathcal{O}(e^{-2\Delta t_{\rm sep}}).
\end{aligned}
} \tag{5}
$$

# Fit models

1. Single-state (plain) summation method fits to individual observables:

$$S(t_{\rm sep}, t_{\rm ex} = a) = C_0 + C_1(t_{\rm sep} - 1)\,, \tag{6}$$

where $C_1 = M_{00}$ and we choose $M_\pi t_{\rm sep}^{\rm min} \geq 0.7$ and $t_{\rm sep}^{\rm min} \geq 0.5\,{\rm fm}$.

2. Simultaneous two-state summmation method fits **(our preferred model):**

$$S(t_{\rm sep}, t_{\rm ex} = a) = M_{00}(t_{\rm sep} - 1) + 2\tilde{M}_{01}\,\frac{e^{-\Delta} - e^{-\Delta t_{\rm sep}}}{1 - e^{-\Delta}}\,, \tag{7}$$

where $\tilde{M}_{01} = M_{01}{\rm Re}\left[\frac{A_1}{A_0}\right]$ and for which we choose $M_\pi t_{\rm sep}^{\rm min} \geq 0.5$.

**NOTE:** Terms $\sim \frac{|A_1|^2}{|A_0|^2}$ are not constrained at our level of statistics and have been dropped.

3. Simultaneous two-state ratio fits (for comparison only):

$$R(t_{\rm ins}, t_{\rm sep}) = c_0 + c_1(e^{-\Delta t_{\rm ins}} - e^{-\Delta(t_{\rm sep} - t_{\rm ins})}) + c_2 e^{-\Delta t_{\rm sep}}\,,$$

where $c_0 = M_{00}$. Here we choose $M_\pi t_{\rm ins}^{\rm min} \gtrsim 0.4$, implying $t_{\rm sep}^{\rm min} = 2t_{\rm ins}^{\rm min}$.

# Some features of summation method based fits

- Results essentially only depend on choice of $t_{\rm sep}^{\rm min}$.
- The choice of $t_{\rm ex}$ has very little impact on the final results.
- All six observables are fitted simultaneously for the two-state summation method (similar to ratio fits):

$\Rightarrow$ **Correlation helps to reduce errors.**

- Dimension of covariance matrix (much) smaller than for ratio based fits at common $t_{\rm sep}^{\rm min}$.

$\Rightarrow$ **Simultanous two-state summation fits are more stable than ratio fits!**

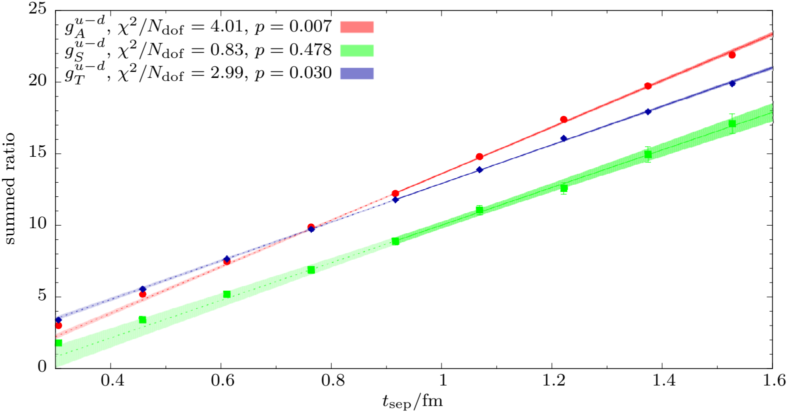
- For a common choice of $t_{\rm sep}^{\rm min}$ the two-state summation fits have a **favorable, leading correction**

$$\sim e^{-\Delta t_{\rm sep}^{\rm min}}$$

compared to the ratio-based two-state fits:

$$\sim e^{-\Delta t_{\rm ins}^{\rm min}} = e^{-\Delta t_{\rm sep}^{\rm min}/2}$$

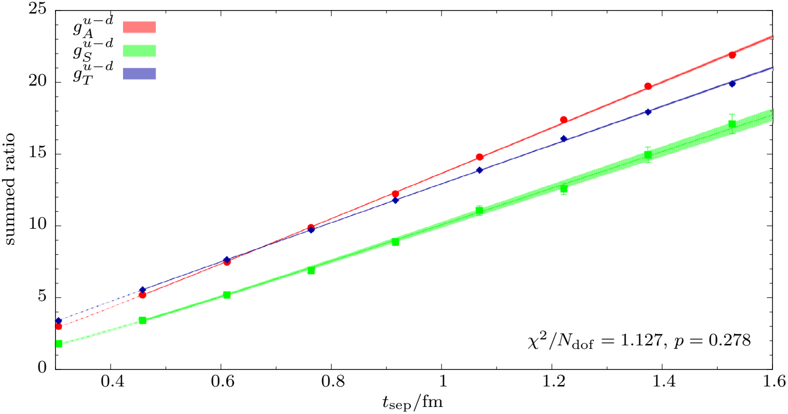
# Single-state vs simultaneous two-state summation method (local NMEs)




Single-state summation method fits for local operator insertions on N451 ensemble ($M_\pi = 286\,\mathrm{MeV}$, $a \approx 0.076\,\mathrm{fm}$).

- Clear deviation from linear behavior at small values of $t_{\rm sep}$.
- Observables are fitted independently.

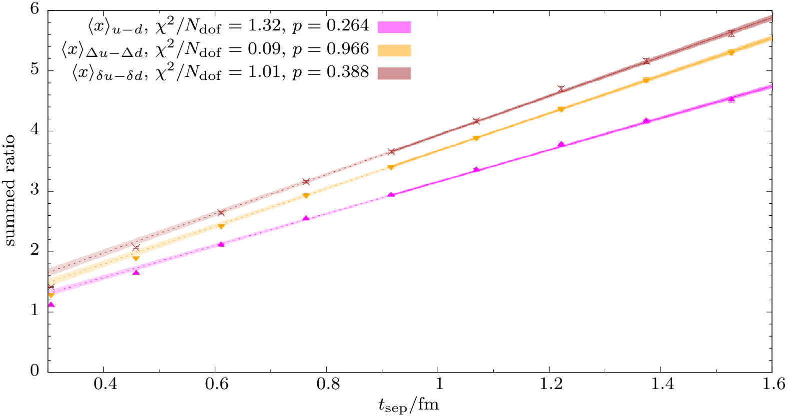
# Single-state vs simultaneous two-state summation method (local NMEs)




Simultaneous two-state summation method fits for local operator insertions on N451 ensemble ($M_\pi = 286\,\mathrm{MeV}$, $a \approx 0.076\,\mathrm{fm}$).

- Data described well by two-state fit to much smaller $t_{\rm sep}$.
- **All six observables are fitted simultaneously.**

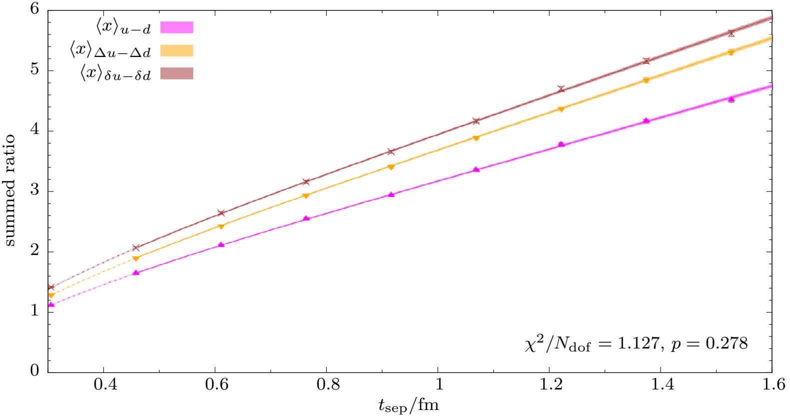
# Single-state vs simultaneous two-state summation method (twist-2 NMEs)




Single-state summation method fits for twist-2 operator insertions on N451 ensemble ($M_\pi = 286\,\mathrm{MeV}$, $a \approx 0.076\,\mathrm{fm}$).

- Deviation even stronger at small $t_{\rm sep}$ than for local operators.
- Larger (relative) errors compared to axial and tensor charge.

# Single-state vs simultaneous two-state summation method (twist-2 NMEs)




Simultaneous two-state summation method fits for twist-2 operator insertions on N451 ensemble ($M_\pi = 286\,\mathrm{MeV}$, $a \approx 0.076\,\mathrm{fm}$).

- Again, data described very well by the two-state fit.
- However, the fit quality rapidly deteriorates including the next smaller $t_{\rm sep}$!

# Chiral, continuum and finite size (CCF) fit model

We consider the following CCF fit model

$$O(M_\pi, a, L) = A_O + B_O M_\pi^2 + C_O M_\pi^2 \log M_\pi + D_O a^{n(O)} + E_O M_\pi^2 e^{-M_\pi L},$$

where

- $n(O) = \begin{cases} 2 & \text{if } O = g_A, g_S \\ 1 & \text{else} \end{cases},$
- $A_O$, $B_O$, $C_O$, $D_O$ and $E_O$ are free fit parameters.

For the axial charge the coefficient $C_{g_A}$ is known analytically, i.e.

$$C_{g_A} = \frac{-\mathring{g}_A}{(2\pi f_\pi)^2}\left(1 + 2\mathring{g}_A^2\right).$$

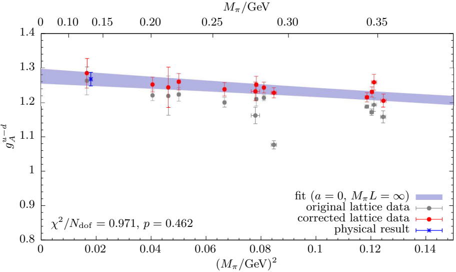
- However: Fitting a free parameter $C_{g_A}$ for $g_A$ gives the “wrong” sign (with large error).
- In general, our data do not constrain a chiral log term, hence we set $C_O = 0$ in our fits.

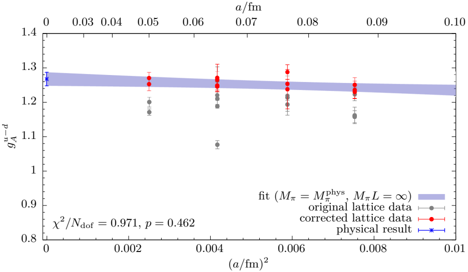
We use $t_0$ to set the scale, with

$$\sqrt{8t_0^{\mathrm{phys}}} = 0.415(4)_{\mathrm{stat}}(2)_{\mathrm{sys}}\,\mathrm{fm}.$$

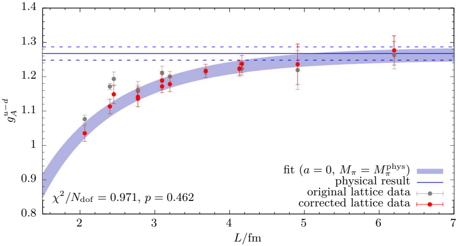
*JHEP 08 (2010) 071*
*Phys. Rev. D95 (2017) 074504*

# CCF for $g_A^{u-d}$ from two-state summation method

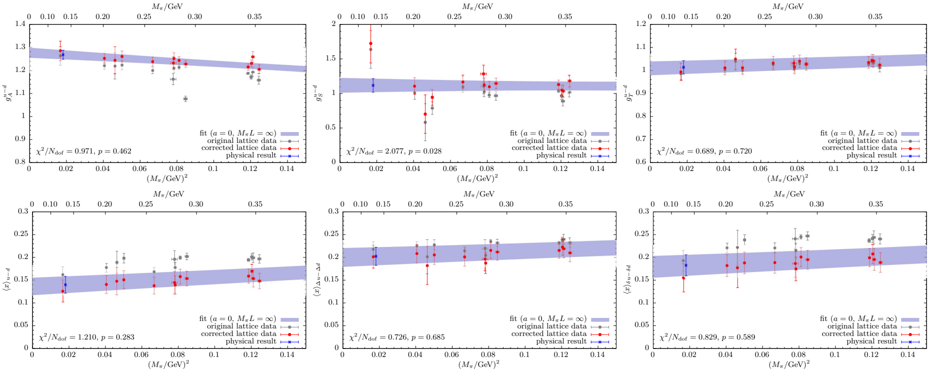



- Data are very well described by the fit model.
- Chiral and continuum extrapolations are mild.
- Large finite volume corrections.
  (already seen in old analysis).
- Physical result in good agreement with result on E250.



# Chiral extrapolation – all observables from two-state summation method




- Chiral extrapolation for all six observables are rather mild.
- Data are generally well described by the fit.
- Large finite volume corrections only seen for $g_A^{u-d}$
- For $\langle x \rangle_{u-d}$ and $\langle x \rangle_{\delta u - \delta d}$ all three extrapolations "conspire" to give downwards shift.

# Preliminary results and outlook

| | $g_A^{u-d}$ | $g_S^{u-d}$ | $g_T^{u-d}$ | $\langle x \rangle_{u-d}$ | $\langle x \rangle_{\Delta u - \Delta d}$ | $\langle x \rangle_{\delta u - \delta d}$ |
|---|---|---|---|---|---|---|
| old analysis (2019) | 1.242(25) | 1.13(11) | 0.965(38) | 0.180(25) | 0.221(25) | 0.212(32) |
| sum. 1-state | 1.258(17) | 1.058(96) | 0.969(27) | 0.136(11) | 0.193(13) | 0.179(15) |
| sum. 2-state | 1.267(19) | 1.118(97) | 1.013(28) | 0.140(18) | 0.203(20) | 0.182(23) |
| ratio fit 2-state | 1.189(23) | 1.147(80) | 0.942(41) | 0.166(32) | 0.179(26) | 0.191(36) |

- Errors in table are statistical only and all new results are preliminary.
- **Summation method-based fits give competitive stat. errors including data at $t_{\mathrm{sep}} < 1\,\mathrm{fm}$**
- Errors from summation method with $t_{\mathrm{sep}} \gtrsim 1\,\mathrm{fm}$ in 2019 analysis were a factor $\sim 4$ larger.
- Computational overhead of additional source-sink separations is small ($\mathcal{O}(20\%)$ of total cost).
- **Suppression of excited state contamination seems improved for summation method based fits.**

**OUTLOOK:**

- Data for an additional ensemble (D452) with $M_\pi \approx 160\,\mathrm{MeV}$ and $N_{\mathrm{meas}} = 128000$ are being generated.
- Increase statistics on E250 (at physical quark mass).
- Include additional, intermediate ("odd") values of $t_{\mathrm{sep}}$ at coarser lattices (?)
- Full assessment of systematic errors due to CCF and residual excited state contamination.