Multi-hadron-state contamination in nucleon observables from chiral perturbation theory

Oliver Bär

Humboldt-Universität zu Berlin

Lattice 2017

Granada

Outline

- Motivation:
  Excited-state contamination in lattice QCD with physical pion mass
- ChPT application:
  Estimate contamination of multi-particle states involving light pions
- Explicitly: ChPT results for $N\pi$-state contribution to lattice estimates for
  - nucleon charges: g_A g_S g_T
  - moments of PDFs: $\langle x \rangle_{u-d}$ $\langle x \rangle_{\Delta u-\Delta d}$ $\langle x \rangle_{\delta u-\delta d}$
- Comparison with lattice data
- ToDo list and Summary

Details in

O. Bär, Phys. Rev. D 92 (2015) 074504
O. Bär, Phys. Rev. D 94 (2016) 054505
O. Bär, Phys. Rev. D 95 (2017) 035506

Simple example: Nucleon 2-pt function

- Consider the nucleon 2-pt function $C_2(t) = \sum_{\vec{x}} \langle N(\vec{x},t)\overline{N}(0,0)\rangle$
  - Σ_x : projection to zero momentum
  - N : interpolating field, quantum numbers of the nucleon

- Spectral decomposition and large time separations
  (Note: finite volume ⇒ discrete spectrum)

➥ $$C_2(t) = b_0 e^{-M_N t} + b_1 e^{-E_1 t} + b_2 e^{-E_2 t} \ldots$$

excited-state contribution

b_0: $|\langle 0|N(0,0)|N(\vec{p}=0)\rangle|^2$

➥ $$M_{\text{eff}}(t) = M_N + \frac{b_1}{b_0}\Delta E_1\, e^{-\Delta E_1 t} + \frac{b_2}{b_0}\Delta E_2\, e^{-\Delta E_2 t} + \ldots$$

effective mass

⇒ time separation needs to be sufficiently large for small excited-state corrections

Excited states in the nucleon sector

- Excited states contributing to the nucleon 2-pt function:
  - Resonance states: $N^*(1440)$, $N^*(1710)$, ...
  - Multi-particle states: $N\pi$, $N\pi\pi$, $\Delta\pi$, ...

- Multi-particle states become important for physical pion masses

Sketch:

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Sketch:

ignore interaction

Finite volume, periodic bc $\quad M_{\pi,\text{phys}} L = 4 \quad \# N(\vec{p}_k)\pi(-\vec{p}_k) = 3$

⇒ discrete momenta

$$\vec{p}_k = \frac{2\pi}{L}\vec{k}$$

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Sketch:

ignore interaction

Finite volume, periodic bc

$\Rightarrow$ discrete momenta

$$\vec{p}_k = \frac{2\pi}{L}\vec{k}$$

$M_{\pi,\mathrm{phys}} L = 4$ $\quad\#N(\vec{p}_k)\pi(-\vec{p}_k) = 3$ ◆

$M_{\pi,\mathrm{phys}} L = 6$ $\quad\#N(\vec{p}_k)\pi(-\vec{p}_k) = 7$ ◆

Excited states in the nucleon sector

$$M_{\text{eff}}(t) = M_N + \frac{b_1}{b_0}\,\Delta E_1\, e^{-\Delta E_1 t} + \frac{b_2}{b_0}\,\Delta E_2\, e^{-\Delta E_2 t} + \ldots$$

- Expectation:
  Many multi-particle states contribute in physical point simulations and dominate at large time separation

- However: Their relevance depends also on the prefactors b_k/b_0
  Known: $b_k \propto 1/L^3$
  BUT: <u>not</u> a FV effect, number of states increases for larger volumes

Other observables:
Nucleon charges and moments of pdfs

- Charges/moments refer to nucleon matrix elements $\langle N(\vec{p})\,|\,O_X(0)\,|N(\vec{p})\,\rangle$ with local quark bilinears O_X

- Nucleon charges:
  - Axial charge g_A: precisely known from neutron beta decay, $g_A/g_V = 1.2723(23)$
    Benchmark observable in Lattice QCD PDG 2015
  - Scalar and tensor charge g_S, g_T : poorly known
    Revived interest in these charges in the context of BSM physics Bhattacharya et al 2012

- Mellin moments of parton distribution functions:
  related to one-derivative operators

Example: $O_X \rightarrow V^a_{\mu\nu} = \overline{u}\gamma_{\{\mu}D^-_{\nu\}}u - \overline{d}\gamma_{\{\mu}D^-_{\nu\}}d \qquad D^-_\mu = (\overrightarrow{D}_\mu - \overleftarrow{D}_\mu)/2$

gives *average quark momentum fraction* $\langle x \rangle_{u-d}$

Analogously: *helicity moment* $\langle x \rangle_{\Delta u-\Delta d}$ and the *transversity moment* $\langle x \rangle_{\delta u-\delta d}$

Lattice determination of axial charge g_A

- In principle: (axial charge, analogous for other charges and moments)

  A) Compute the 3-pt function

$$C_3(t,t') = \sum_{\vec{x},\vec{y}} \Gamma_k \langle N(\vec{x},t)\, A_k^3(\vec{y},t')\, \overline{N}(\vec{0},0)\rangle$$

axial vector current

gamma matrix, properly chosen

  B) Form ratio with 2-pt function

$$R_A = \frac{C_3(t,t')}{C_2(t)}$$

and consider large time separations

excited-state contribution

$$R_A \xrightarrow{t \gg t' \gg 0} g_A + \tilde{b}_1\, e^{-\Delta E_1 (t-t')} + \tilde{b}_1' e^{-\Delta E_1 t'} + \tilde{c}_1 e^{-\Delta E_1 t} + \ldots$$

  C) Obtain axial charge from a fit to lattice data for R_A

  Plateau method, Summation method → later

- In practice: smaller time separations t-t' and t' than in 2-pt function

  ➡ less exponential suppression and larger excited-state contributions

$N\pi$ contribution in ChPT

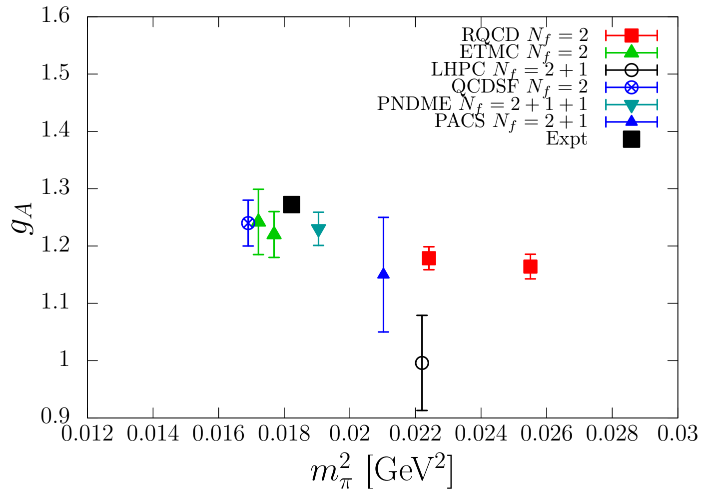
$$R_A = \; g_A + \tilde{b}_1\, e^{-\Delta E_1(t-t')} + \tilde{b}_1' e^{-\Delta E_1 t'} + \tilde{c}_1 e^{-\Delta E_1 t} + \ldots$$

- In the following: Compute the 2pt and 3pt functions and the ratios in ChPT
  - ➡ Provides the contribution due to $N\pi$ states
    which is expected to dominate for large time separations
- Not a new idea
  Tiburzi 2008; OB, Golterman 2013
- Note: The leading order results for the $N\pi$ contribution
  to all charges and moments are related
  Chiral symmetry at work !

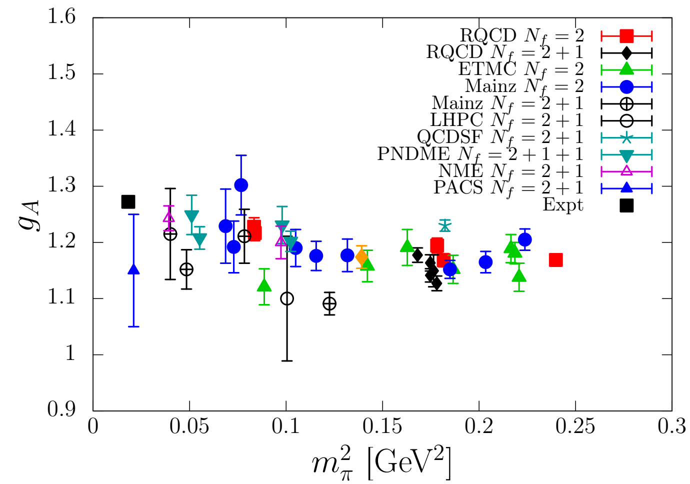
Lattice results for g_A - Status 2016

Isovector charges g_A

Several $m_\pi < 165$ MeV results.



Impose $Lm_\pi > 4$, $a < 0.1$ fm



ETMC: [Alexandrou,Mon,15:15] $N_f = 2$ twisted mass fermions, $Lm_\pi = 3$. Increased statistics on 1507.04936, 579 configs $\times$ 16 measurements, $g_A = 1.22(3)(2)$ - systematics from fitting.

PACS: [Kuramashi,Thu,16:30] $N_f = 2+1$ NP clover, stout smeared links, $m_\pi = 145$ MeV, $a = 0.085$ fm, 146 configs $\times$ 64 measurements, $t_f - t_i$=1.3 fm, $Lm_\pi = 6$

PNDME: [Gupta,Thu,17:50]

Sara Collins' talk, Lattice 2016

Chiral Perturbation Theory (ChPT)

- Well-known and widely used in Lattice QCD

ChPT: low-energy effective theory of QCD

Weinberg 1979,
Gasser, Leutwyler 1983,
Gasser, Sainio, Švarc 1988,
Becher, Leutwyler 1998,
…

- Many applications of Baryon ChPT

review: V. Bernard, Prog. Part. Nucl. Phys. 60 (2008) 82-160

  - Nucleon-pion scattering, nucleon form factors, …
  - Pion mass dependence of nucleon observables
  - FV effects due to pions
  - …

ChPT including nucleons

- SU(2) ChPT at LO

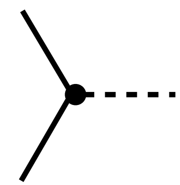
  Gasser, Sainio, Švarc 1988

  isospin symmetry, euclidean space time

  contains the three pions and the nucleon doublet $\Psi = \begin{pmatrix} p \\ n \end{pmatrix}$

$$\mathcal{L}^{(1)}_{\mathrm{int},1\pi} = \frac{ig_A}{2f}\overline{\Psi}\gamma_\mu\gamma_5\sigma^a\Psi\,\partial_\mu\pi^a$$

→ nucleon-pion vertex



Note:

- one pion derivative
- 2 LECs: g_A axial charge

  f pion decay constant

  chiral limit values

ChPT including nucleons

Operators in ChPT:

- Known:
  - Axial vector and scalar density for axial and scalar charge g_{A}, g_{S}
    Gasser, Sainio, Švarc 1988, Fettes *et al* 2000
  - Effective operators for $< x >_{u-d}$ and $< x >_{\Delta u-\Delta d}$
    Dorati, Gail, Hemmert 2008, Wein, Bruns, Schäfer, 2014
- Easy to construct (to LO): operators for tensor charge g_T and $< x >_{\delta u-\delta d}$
  (tensor operators at the quark level)
  OB 2016
- Note: The chiral limit values of all charges and moments appear as LECs !
  Input, not predicted by ChPT

ChPT including nucleons

Nucleon interpolating fields in ChPT:

- Standard local 3-quark baryon operators are mapped to ChPT based on their symmetry properties
  Nagata et al 2008; Wein, Bruns, Hemmert, Schäfer 2011

- Holds for smeared interpolating fields too if $R_{\rm smear} \ll \dfrac{1}{M_\pi}$
  Lüscher 2013; OB, Golterman 2014

  Physical pion mass: $R_{\rm smear} \cong$ 0.3 - 0.4 fm seems ok

- Difference between local and smeared fields: different LECs

$N\pi$ contribution in ChPT

- Calculation of the 2pt and 3pt functions is a standard calculation in PT
  in position space and in a finite spatial volume
  (time extent infinite for simplicity)

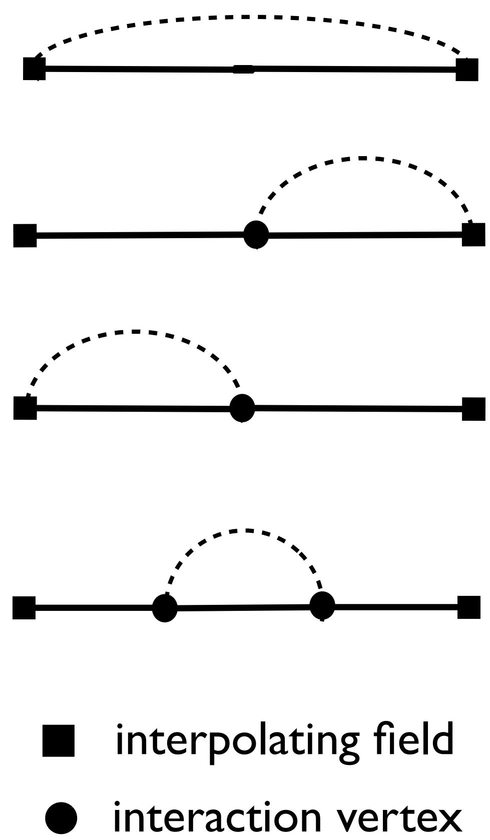
- E.g.: Feynman diagrams for the $N\pi$ contribution in the 2pt-function:

  ➡ Extract contribution with exponential decay given by

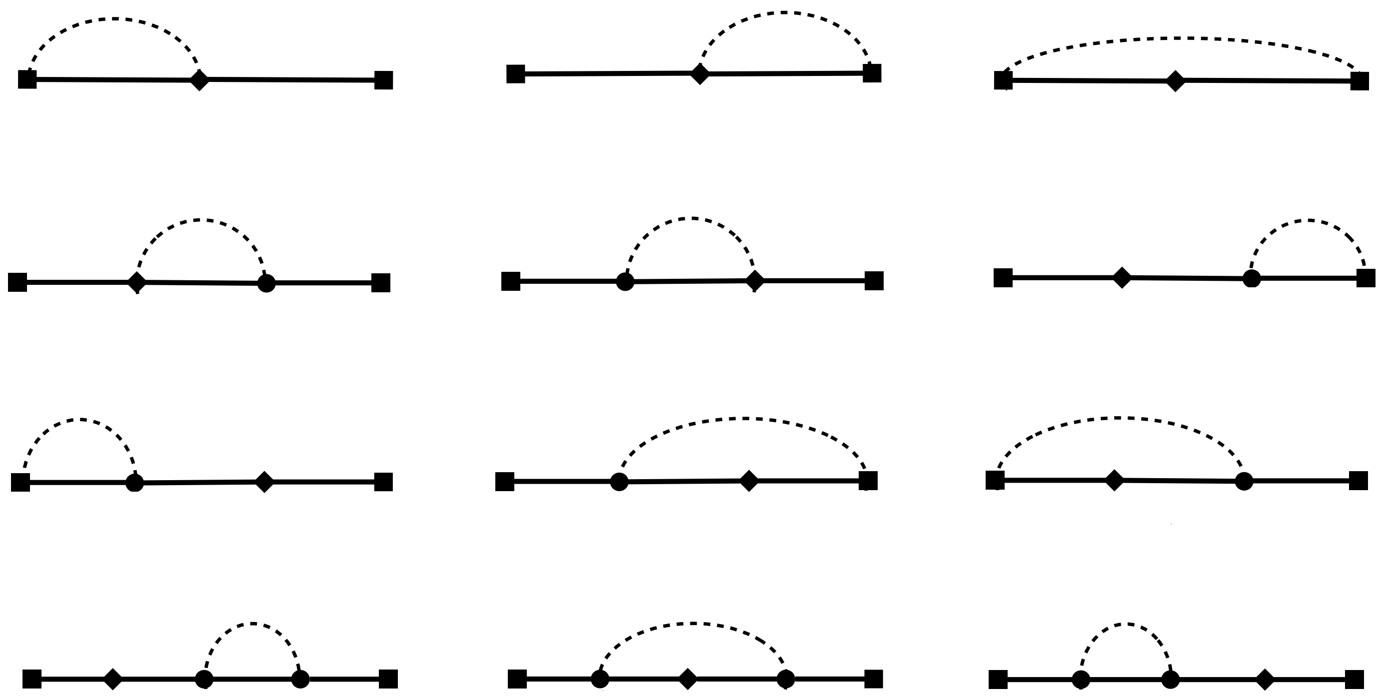
$$E_{\rm tot} = E_N + E_\pi \qquad \vec{p}_N = -\vec{p}_\pi$$

  (ignore other contributions !)

- Note: Tree-level calculation !



Feynman diagrams for the 3pt-functions



■ interpolating field ◆ operator ● interaction vertex

Results: $N\pi$ contribution to ratio R_X

$$R_X(t,t') = g_X\left[1 + \sum_{\vec{p}_n}\left(b_{X,n}e^{-\Delta E_n(t-t')} + b_{X,n}e^{-\Delta E_n t'} + c_{X,n}e^{-\Delta E_n t}\right)\right]$$

$$\Delta E_n = E_{\mathrm{tot},n} - M_N$$

X = A (axial vector), S (scalar density), …

- Non-trivial result of the calculation: The coefficients $b_{X,n}, c_{X,n}$
- Example:

m_n: degeneracy factor $m_1 = 6, m_2 = 12, \ldots$

$$c_{X,n} = \frac{m_n}{16(fL)^2 E_{\pi,n} L}\left(1 - \frac{M_{N,\mathrm{ch}}}{E_{N,n}}\right)\left(\ \cdots\ \right)$$

← not very illuminating …

Note:
- $1/L^3$ suppression of individual coefficients
- vanishes for nucleon/pion at rest (parity!)

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$$\Delta E_n = E_{\mathrm{tot},n} - M_N$$

X = A (axial vector), S (scalar density), …

The coefficients

- do <u>not</u> depend on the LECs associated with the interpolating fields
  no longer true beyond LO
- depend only on
  - pion mass and decay constant
  - the spatial volume via $M_\pi L$
  - four LO LECs: nucleon mass, axial charge, av. mom. fraction and helicity moment
    chiral limit values
- Use exp. / phen. values ⇒ estimate $N\pi$ contribution in lattice simulations

Impact on the plateau estimate

- Plateau / Midpoint estimate for the charges and moments:

$$R_X(t, t' = \frac{t}{2}) \approx g_X + \mathrm{O}(e^{-\Delta E_n \frac{t}{2}}) + \mathrm{O}(e^{-\Delta E_n t})$$

minimises excited-state contribution for a given source-sink separation

- For estimates use experimental values for masses / low-energy constants:

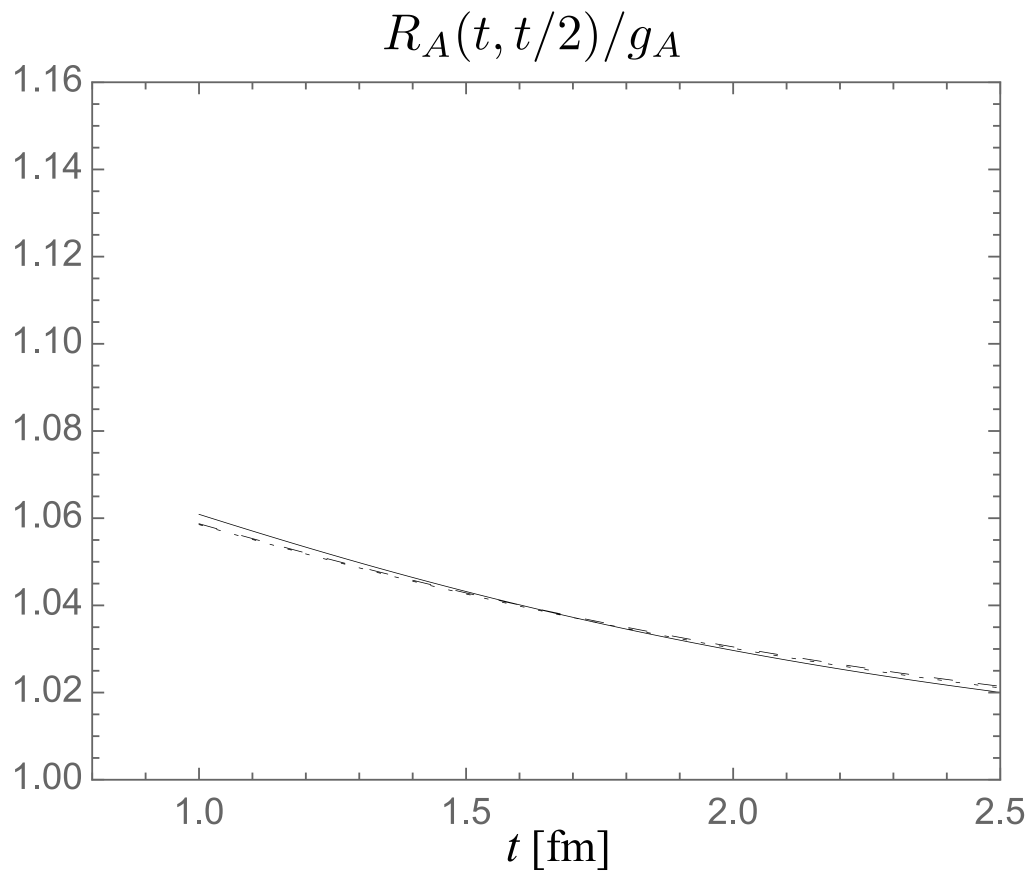
$M_\pi = 140$ MeV $M_N = 940$ MeV

$f_\pi = 93$ MeV $g_A = 1.27$ $\langle x \rangle_{u-d} = 0.165$ $\langle x \rangle_{\Delta u - \Delta d} = 0.19$

PDG 2015
Alekhin et al 2012
Blümlein et al 2010

➥ only the spatial volume remains to be fixed (via $M_\pi L$)

$N\pi$ contribution to plateau estimate for g_A

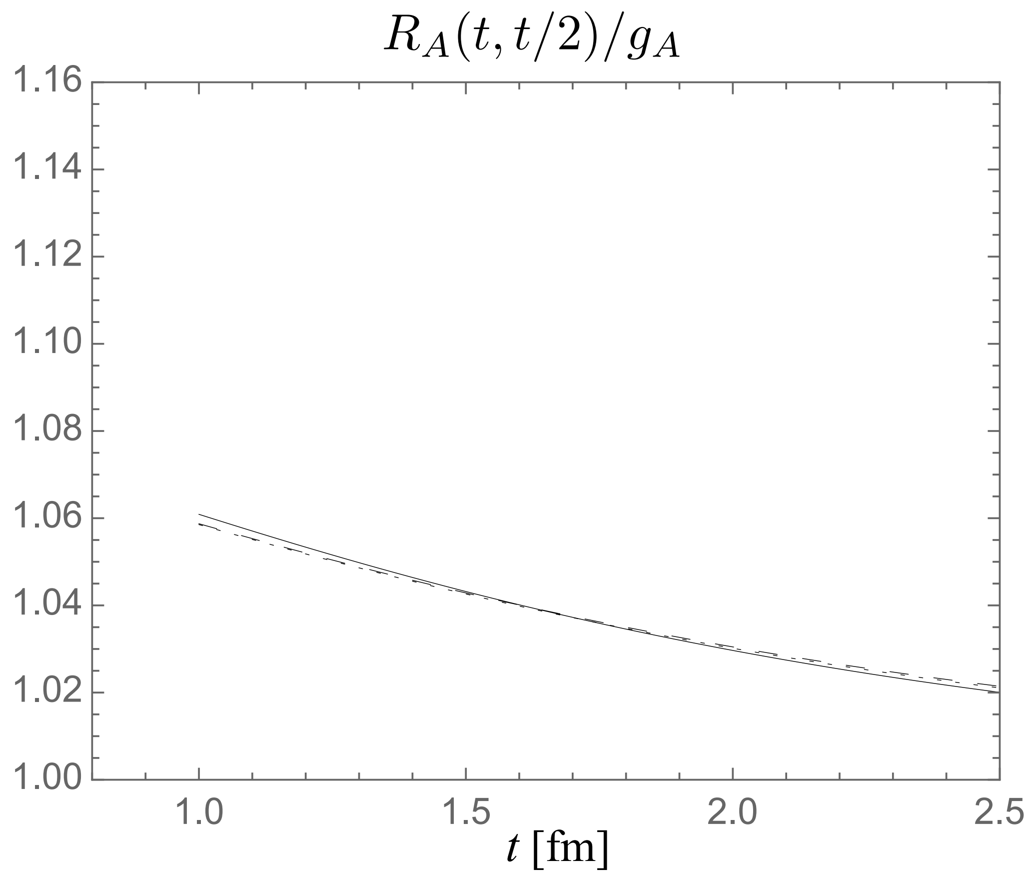


solid: $M_\pi L = 4$

dotted: $M_\pi L = 5$

dashed: $M_\pi L = 6$

$N\pi$ contribution to plateau estimate for g_A



solid: $M_\pi L = 4$

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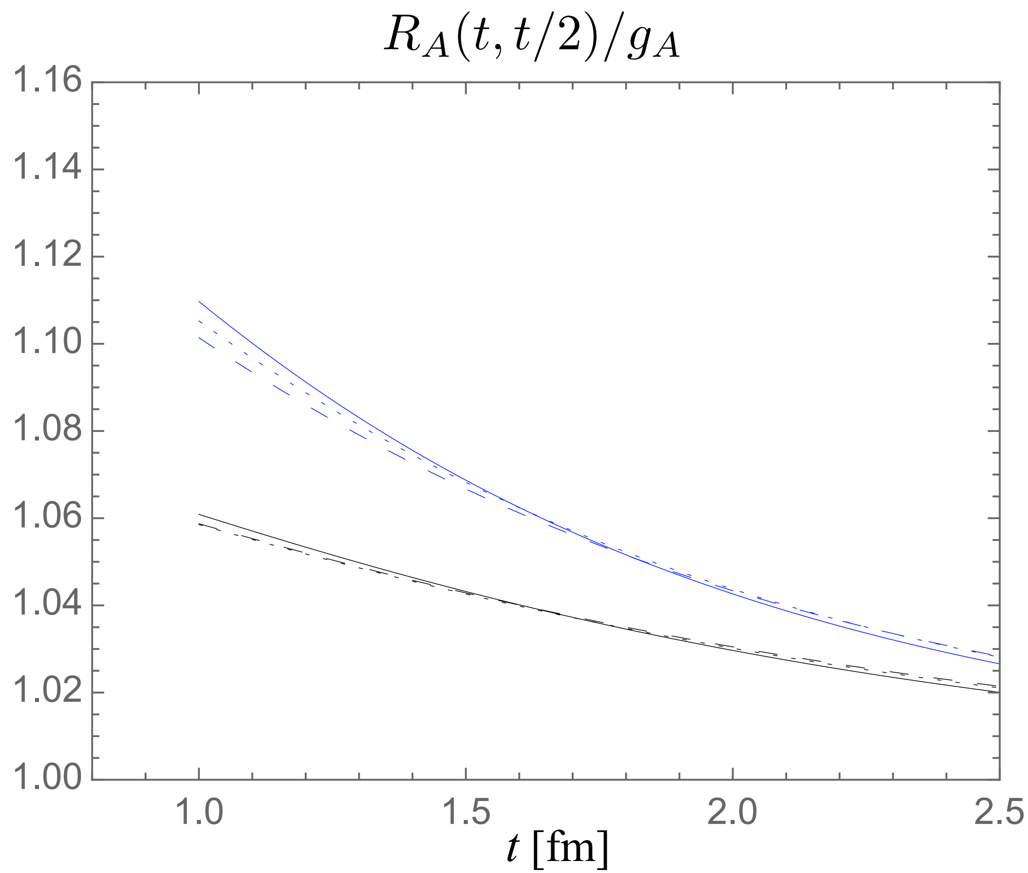
dashed: $M_\pi L = 6$

— $N_{\text{States}} \leq N_1$

$N_{\text{States}}(L)$ such that energy interval is fixed:

$N\pi$ contribution to plateau estimate for g_A



solid: $M_\pi L = 4$

dotted: $M_\pi L = 5$

dashed: $M_\pi L = 6$

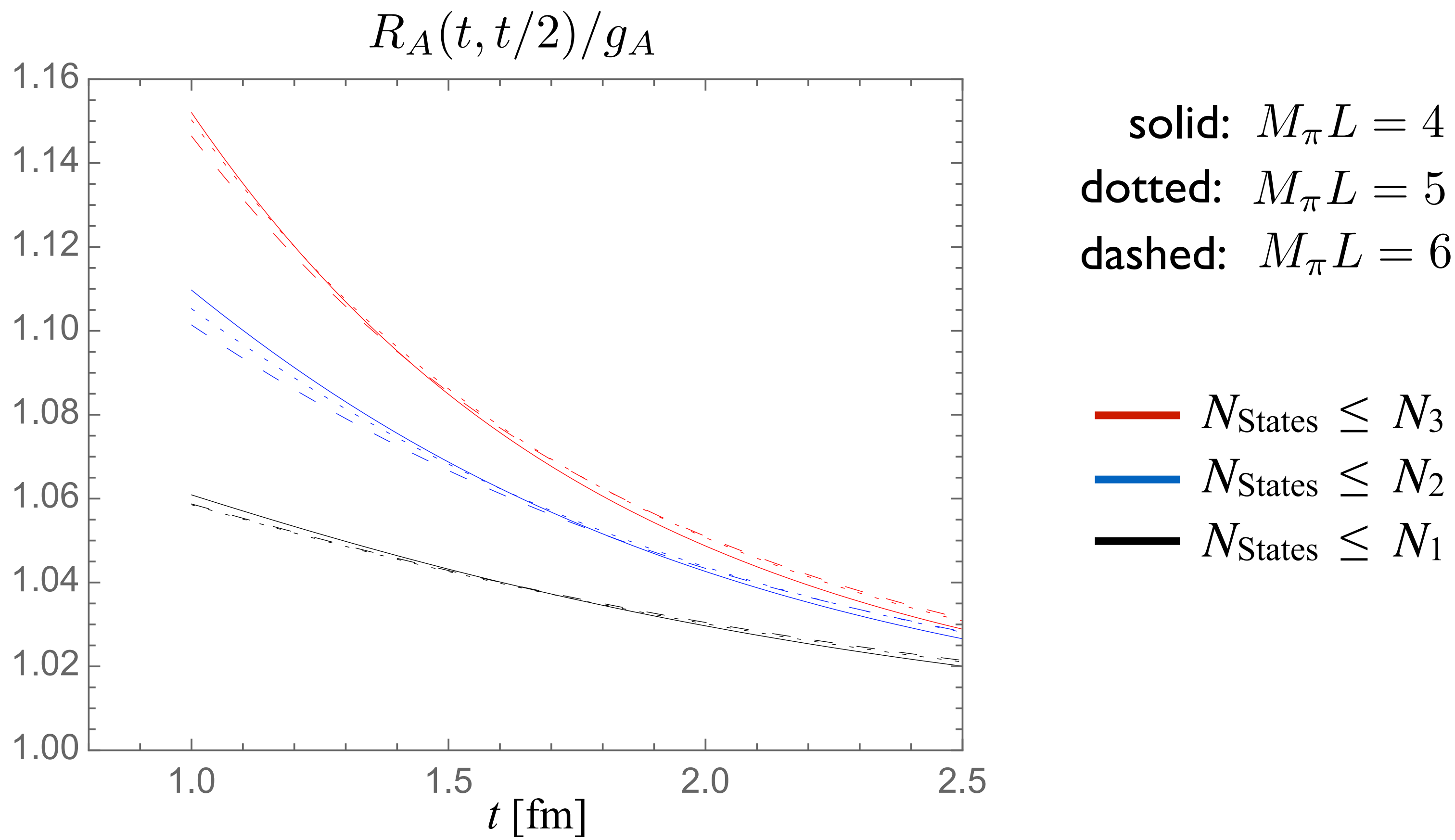
$N_{\text{States}} \leq N_2$

$N_{\text{States}} \leq N_1$

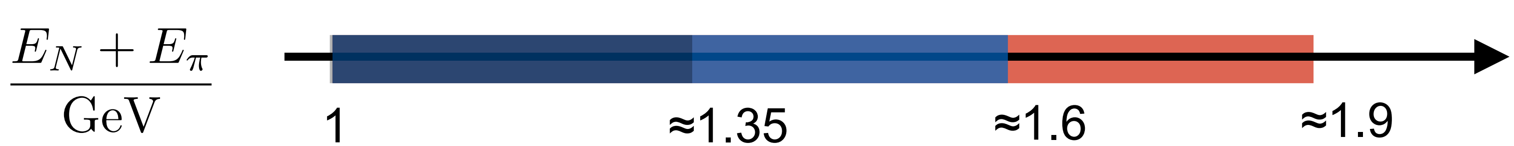
$N_{\text{States}}(L)$ such that energy interval is fixed:

$\frac{E_N + E_\pi}{\text{GeV}}$

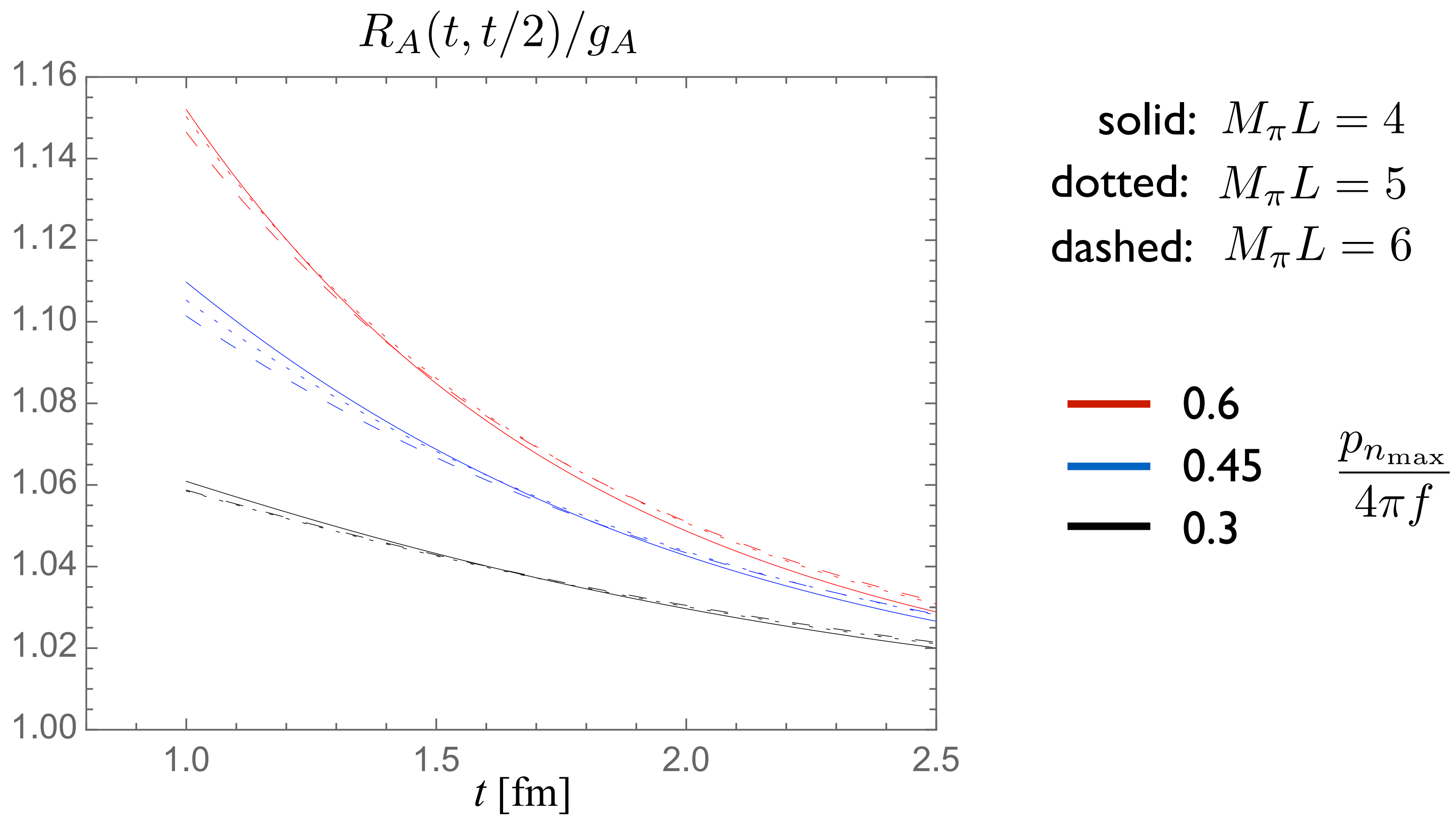
$N\pi$ contribution to plateau estimate for g_A



$N_{\text{States}}(L)$ such that energy interval is fixed:



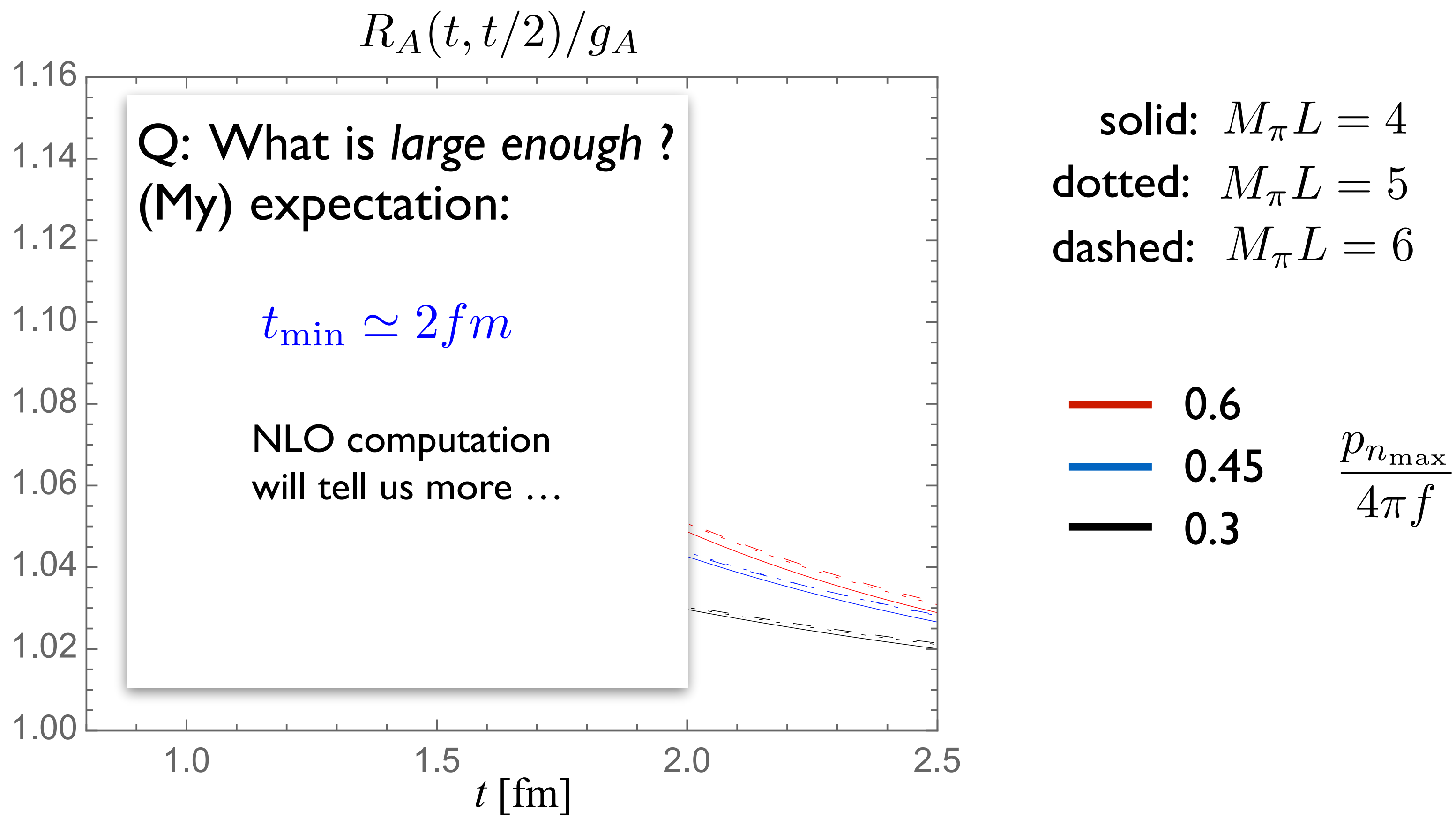
$N\pi$ contribution to plateau estimate for g_A



Conclusion: $N\pi$ contribution leads to an overestimation of the axial charge
But: ChPT is an expansion in small momenta $p_n/4\pi f$

➡ source-sink separation needs to be large enough for high-momentum states to be sufficiently suppressed

$N\pi$ contribution to plateau estimate for g_A



Q: What is *large enough* ?
(My) expectation:

$t_{\min} \simeq 2fm$

NLO computation
will tell us more …

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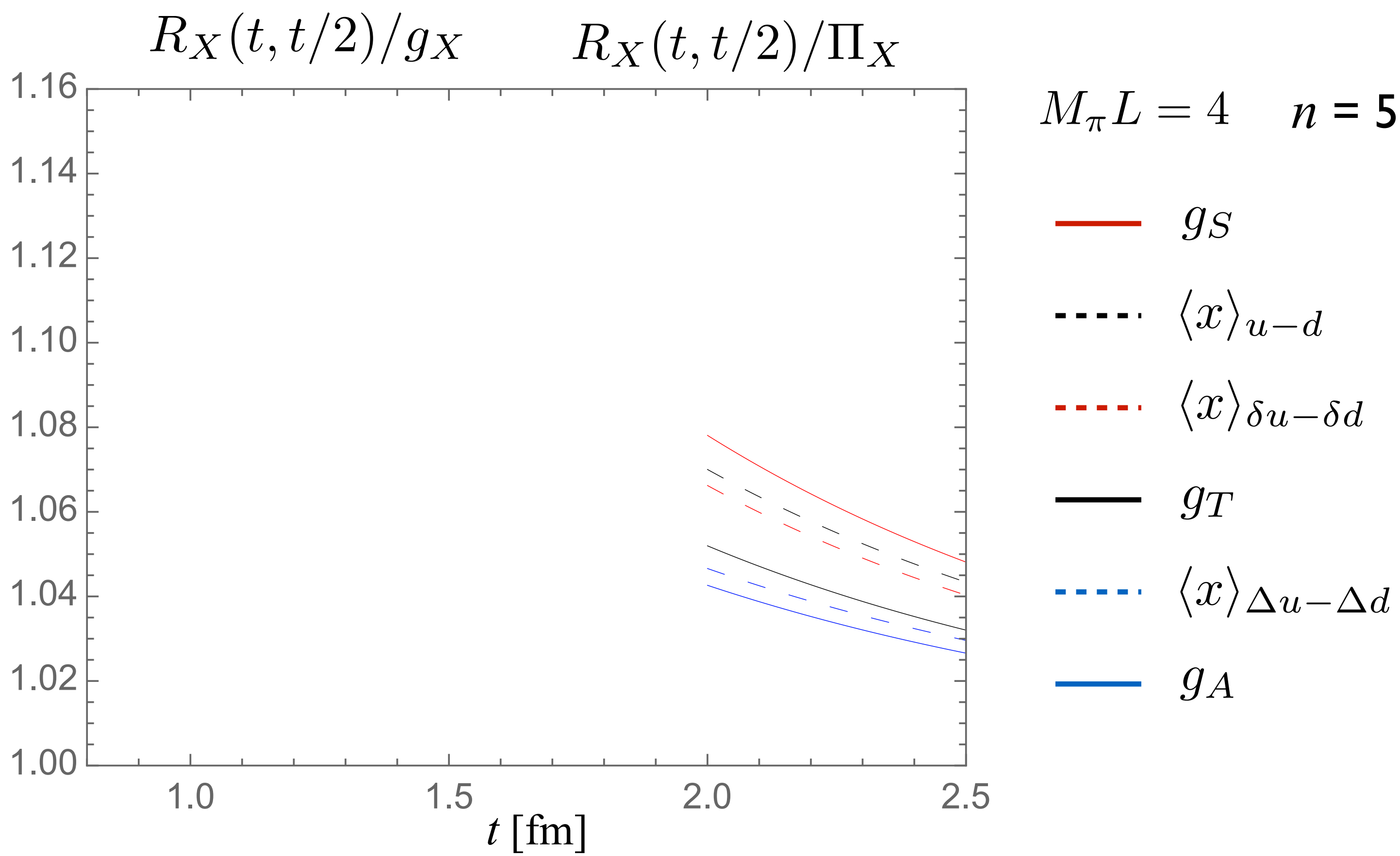
Analogous results for other charges and moments



Analogous results for all charges and the moments:

- Small FV effects
- Small momentum $N\pi$ states start to dominate for $t \gtrsim 2$ fm
- $N\pi$ contribution leads to an overestimation for all charges / moments
- The overestimation is at the 5 - 10% level for $t \approx 2$ fm

Comparison with lattice data ?

- Some collaborations have performed simulations with $M_\pi \lesssim 165$ MeV

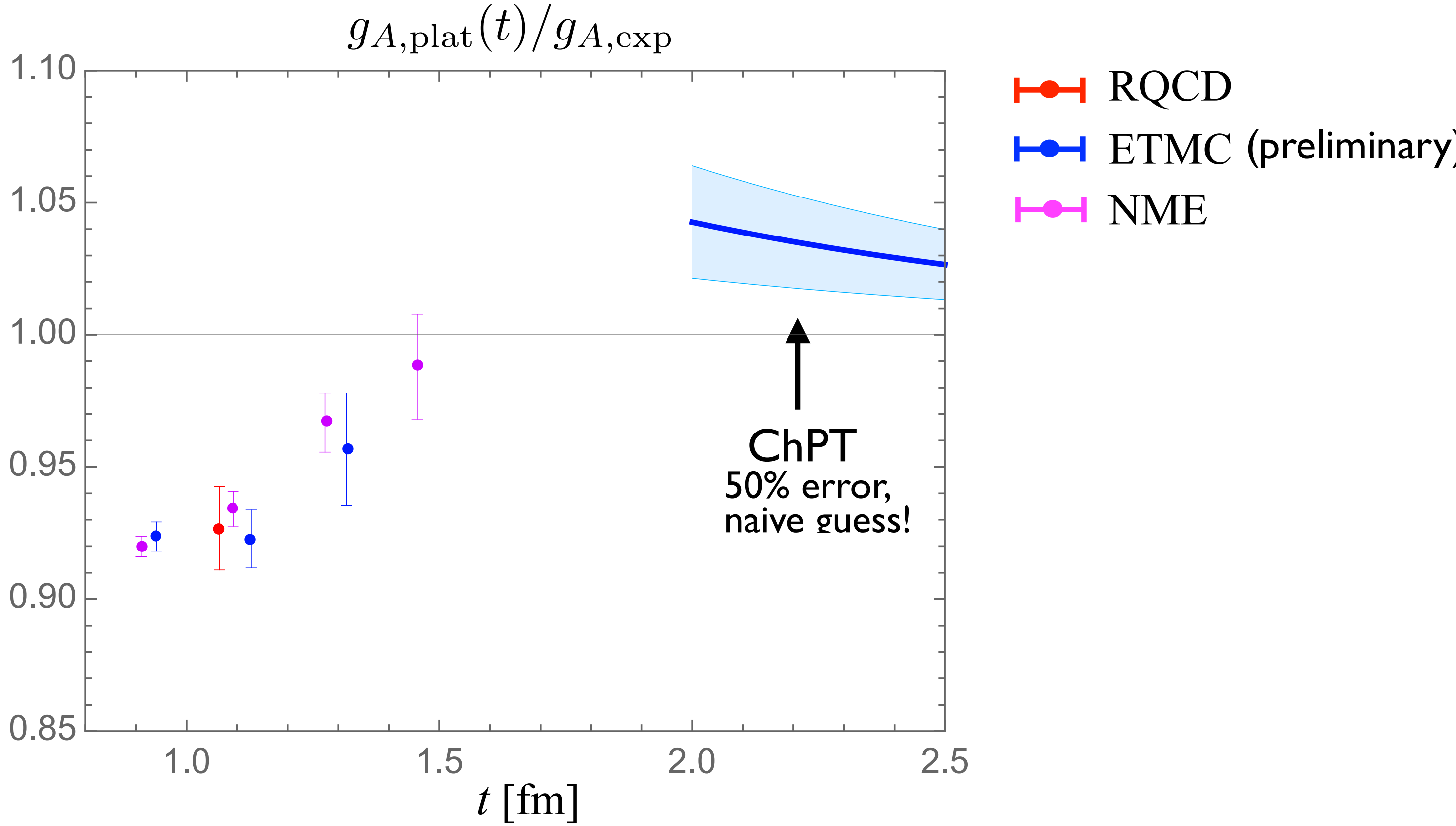
  - RQCD
    $N_f = 2$ NPI Wilson-clover, $a \approx 0.07$ fm, $M_\pi \approx 150$ MeV, $M_\pi L \approx 3.5$
    PRD 90 (2014) 074510
    PRD 91 (2015) 054501

  - ETMC
    $N_f = 2$ WilsonTM-clover, $a \approx 0.09$ fm, $M_\pi \approx 130$ MeV, $M_\pi L \approx 3$
    PRD 92 (2015) 114513
    arXiv:1706.02973

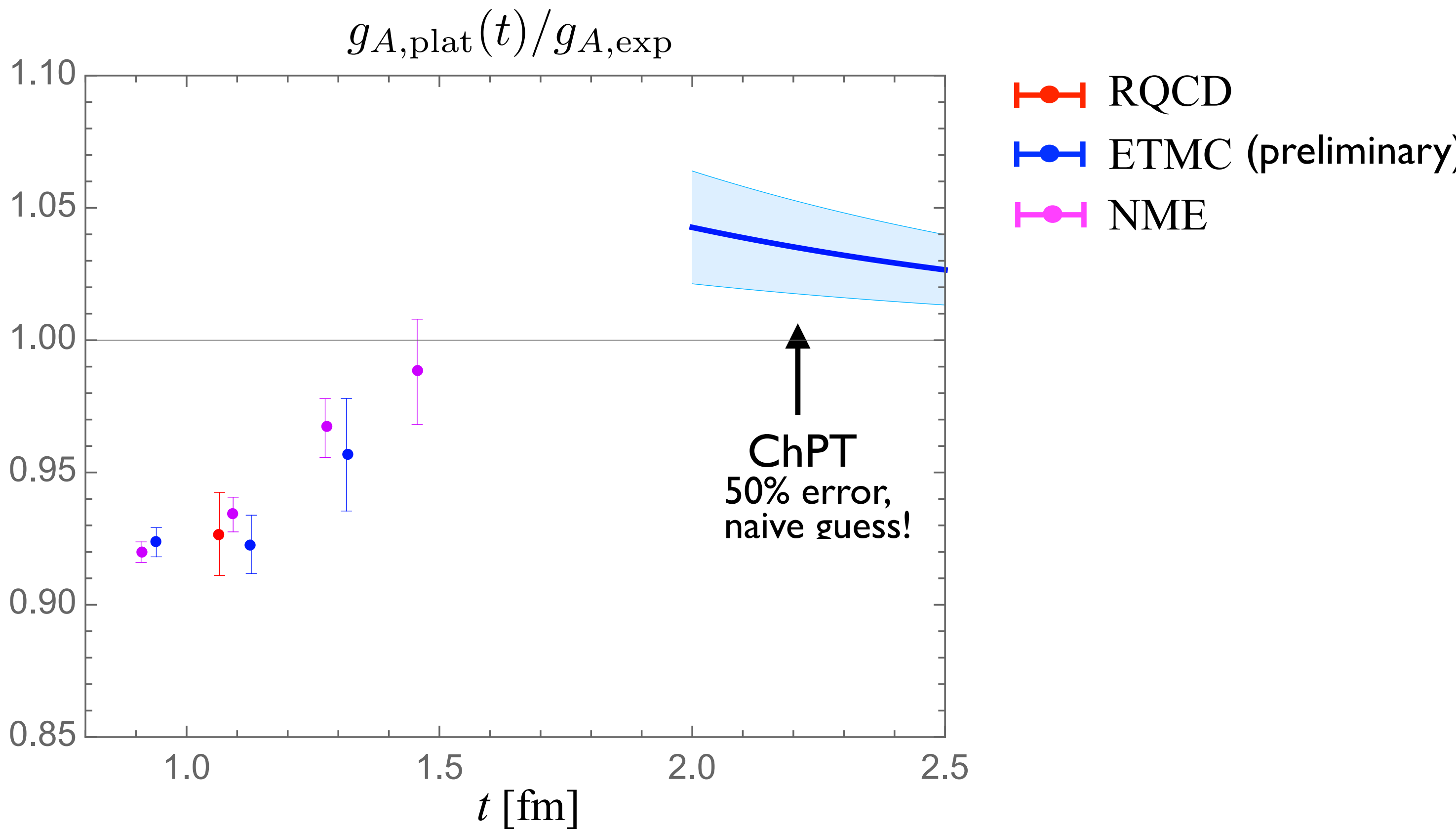
  - NME
    $N_f = 2{+}1$ Wilson-clover, $a \approx 0.09$ fm, $M_\pi \approx 166$ MeV, $M_\pi L \approx 3.7$
    ➜ R. Gupta, Mon, 14:30
    PRD 95 (2017) 074508

- Main obstacle for direct comparison with ChPT results: $t \lesssim 1.5$ fm, too small !

Comparison with lattice data: axial charge



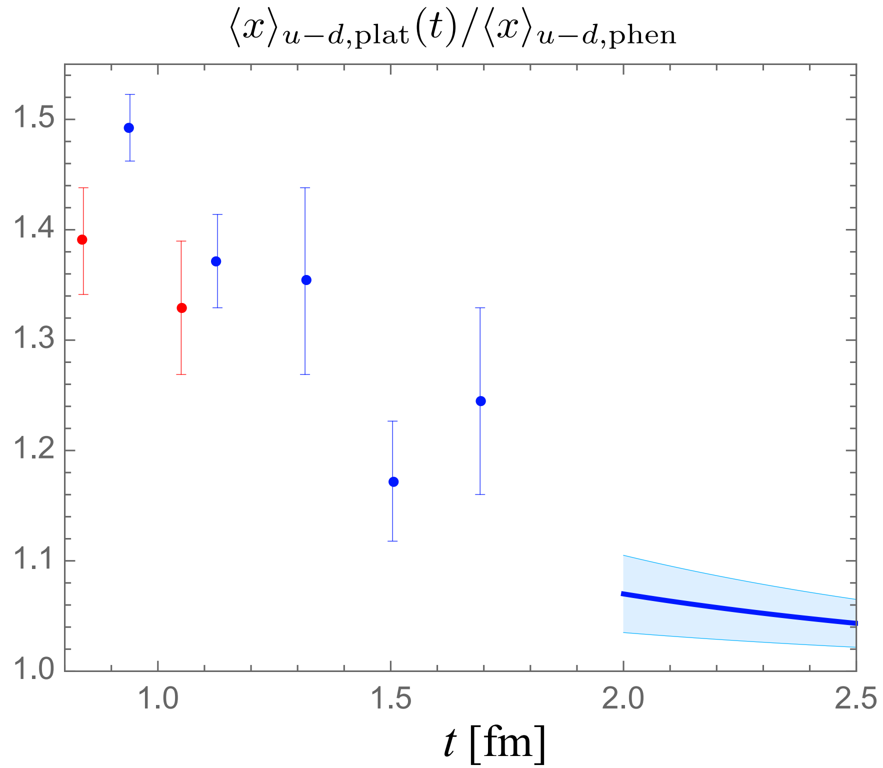
Comparison with lattice data: axial charge

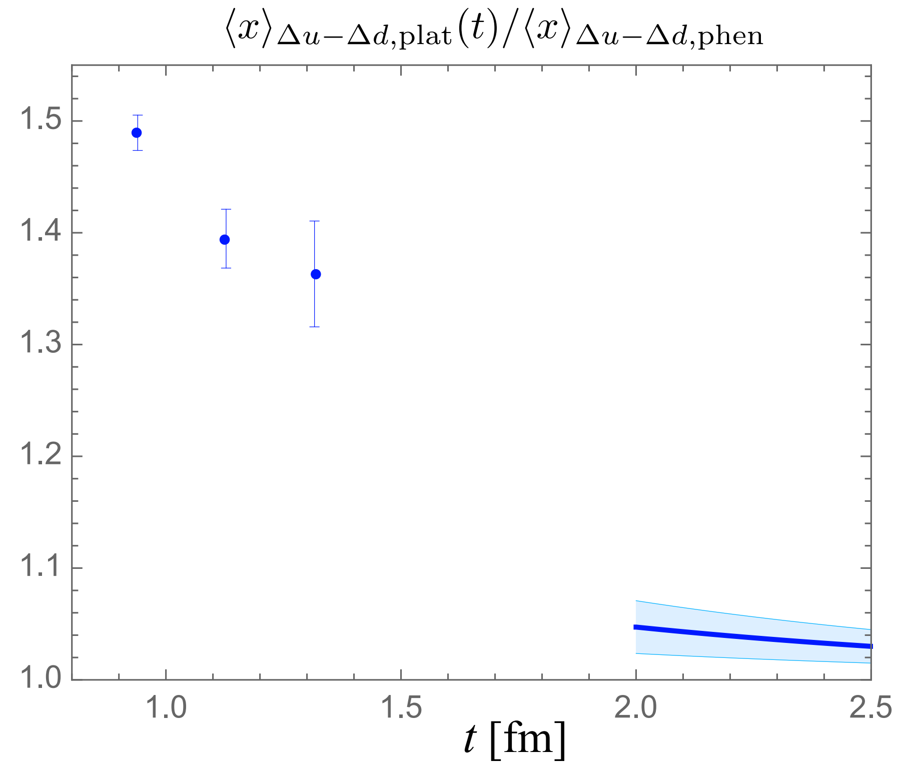


Lattice data + ChPT suggests <u>accidental agreement</u> for some $t \approx 1.5\mathrm{fm}$

➡ needs to be checked !

Comparison with lattice data: average momentum fraction and helicity moment





RQCD

ETMC (prel.)

50% error
for coefficients

Impact on the summation estimate

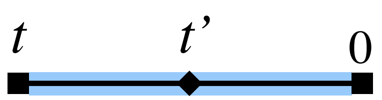
- Summation estimate for the axial charge (analogous for other charges and moments)

$$\sum_{t'=0}^{t} R_A(t,t') \xrightarrow{t \gg 0} t\,[\,g_A + \mathrm{O}(e^{-\Delta E_n t})\,] + \ldots$$

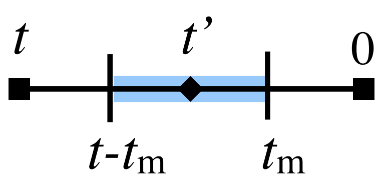
summation estimate

Maiani *et.al.* 1987
Capitani *et.al.* 2012

- Note: involves 3pt-function at short distances
  ➥ not properly captured by ChPT

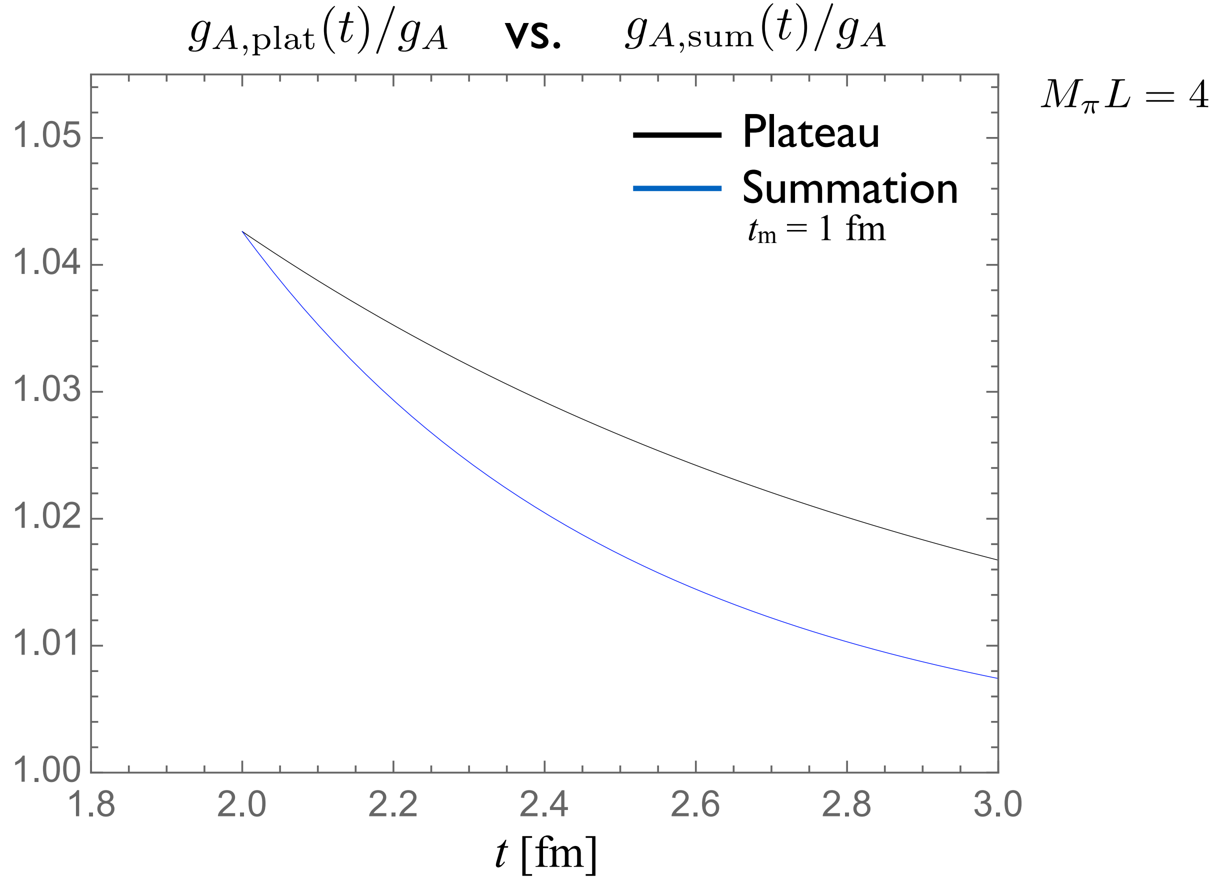


- Remedy: Sum/Integrate over sub-interval only keeping all distances large



➥ even larger source sink separations are needed than for the plateau method

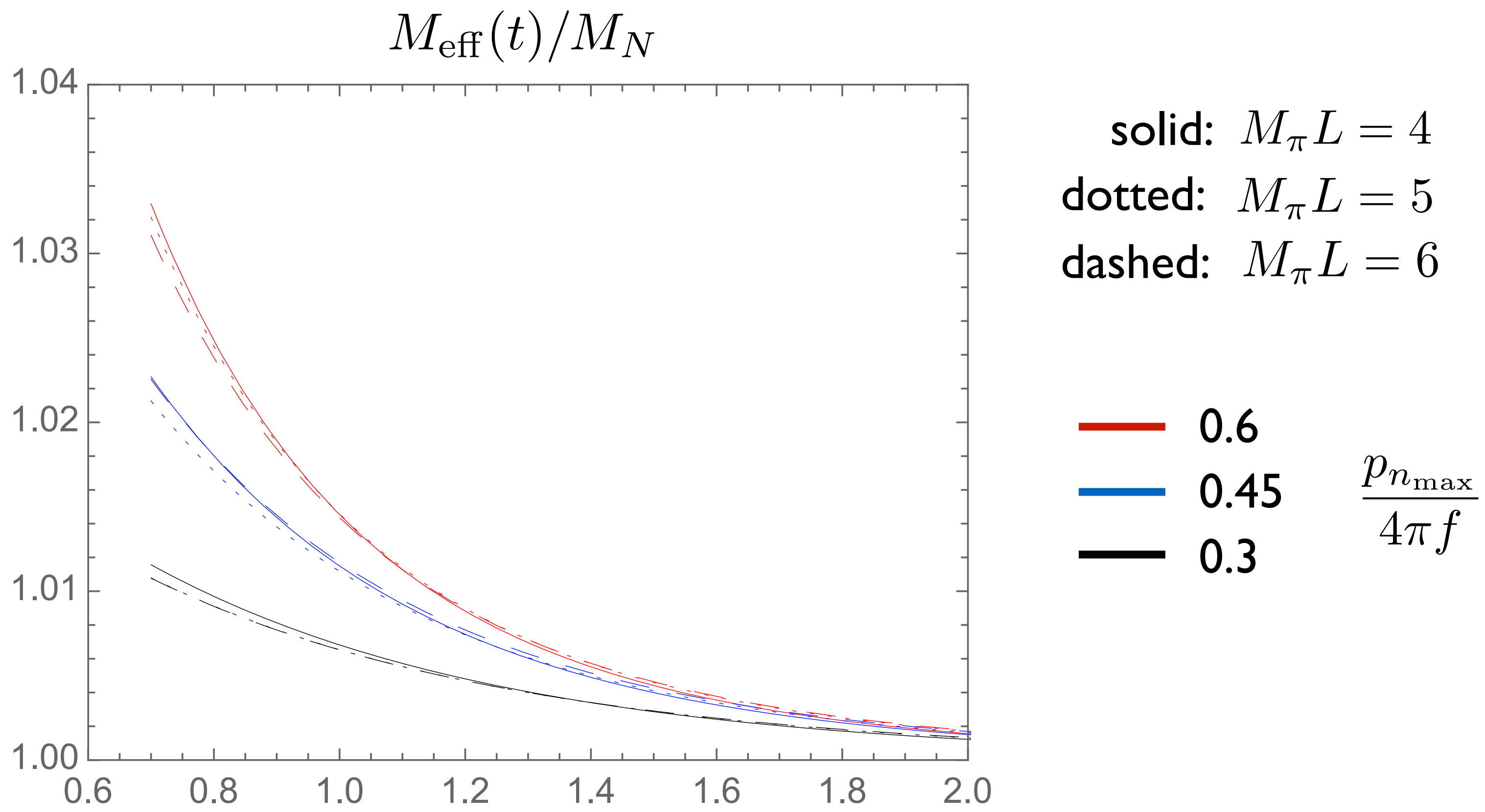
Result: Summation estimate for axial charge



Conclusions:

- Summation estimate is slightly better
- Summation method leads to overestimation too

$N\pi$ contribution to effective nucleon mass



Conclusions:

- Small momentum $N\pi$ states start to dominate for $t \gtrsim 1.2$ fm
- $N\pi$ contribution is well below 2% for $t \gtrsim 1.2$ fm

To do list

- So far: Conclusions based on LO results for $N\pi$-state contribution
- To do
  - Compute/estimate impact of other states: $N\pi\pi$, $\Delta\pi$, N^*
  - Compute $N\pi$ contribution to next order to get a more honest error estimate

Summary

- ChPT can provide estimates for multi-hadron-state contributions in nucleon observables

- Based on LO ChPT: The $N\pi$-state contribution
  - leads to an overestimation of various nucleon charges and pdf moments
  - is at the 5-10% level for these observables

  !!! assuming source-sink separations $t \approx 2$ fm

- Comparison with lattice data suggests that much larger source-sink separations are needed
  - to be in the asymptotic regime with ground state dominance
  - to get the charges/moments with few percent precision

requires new ideas to tackle the signal-to-noise problem ➜ L. Giusti, Mon, 12:00

➜ M. Wagman, Thu, 15:10

Backup slides

Results: Plateau estimate for g_A

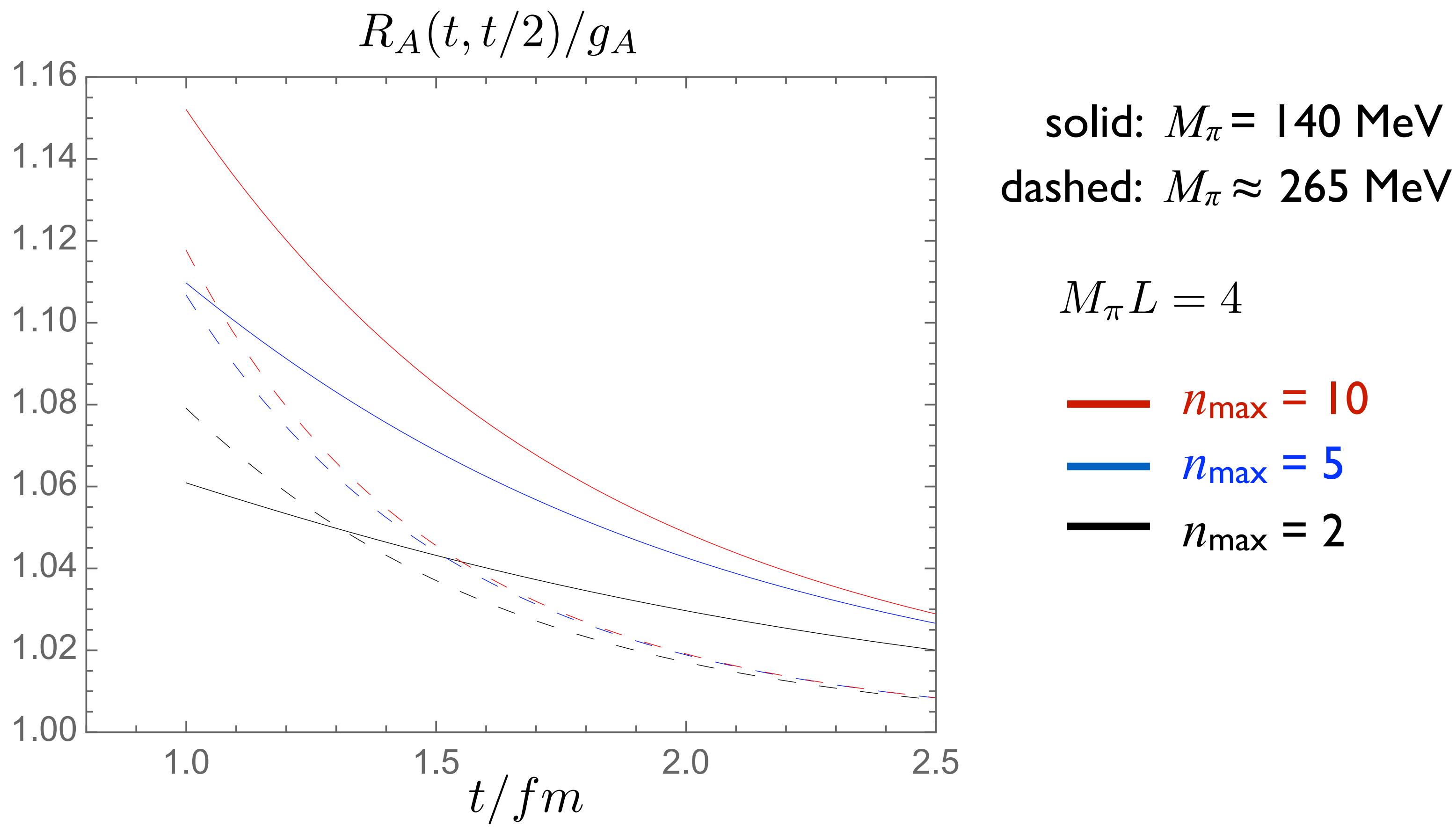
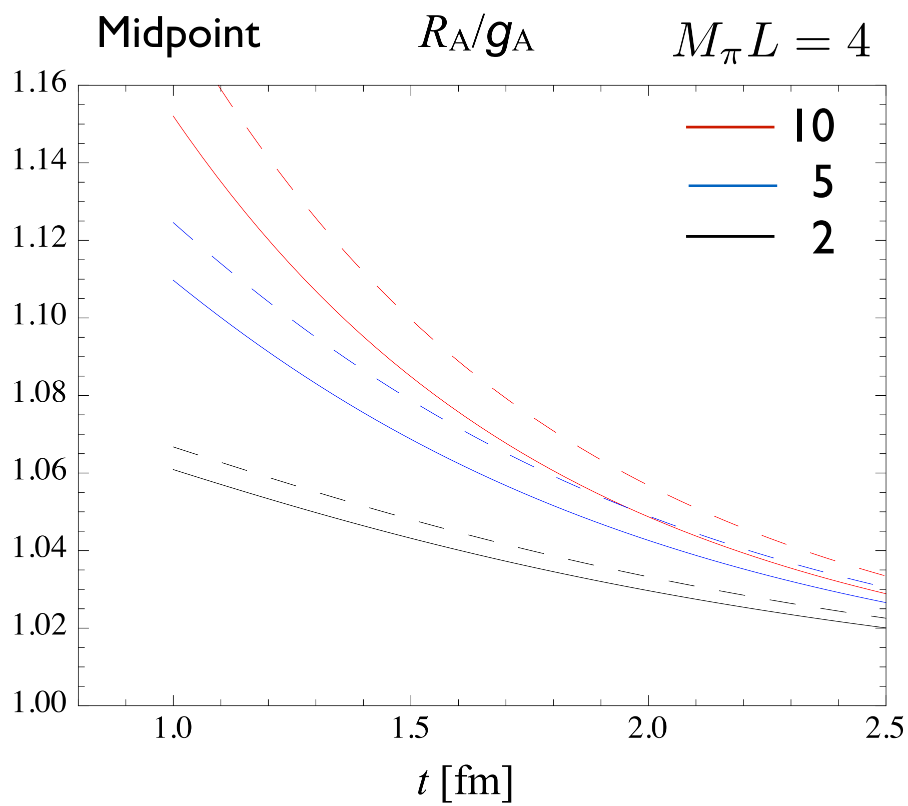


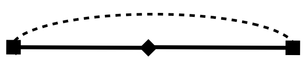
Illustration: heavier than physical pion mass

- $N\pi$ contribution is a factor 2-3 smaller
- dominant contribution stems from smaller number of states for smaller values t

Impact $N\pi$ vertex in interpolating field



dashed lines:
drop $N\pi$ vertex in int.pol. fields
i.e. drop



+ 6 more

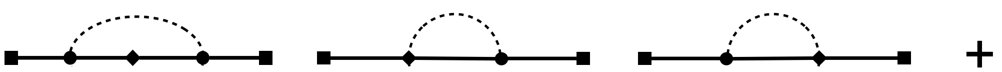
Observation:
$N\pi$ vertex correction to interpolating field has a small impact on the total result
True for higher orders too???

Include finite volume effects

Our result $$R_A = g_{A,\mathrm{ch}}\left[1 + \delta_{\mathrm{N}\pi,g_A}(M_\pi L, M_\pi/M_N)\right]$$

Replace $$g_{A,\mathrm{ch}} \longrightarrow g_A(L) = g_A(\infty)\left[1 + \delta_{\mathrm{FV},g_A}(M_\pi L)\right]$$

stems from 1-loop diagrams shown before



FV correction is known

Ali Khan et al 2006

Horsley et al 2014

$$\delta_{\mathrm{FV},g_A}(M_\pi L) = \delta_{\mathrm{FV},f_\pi}(M_\pi L) + \Delta(M_\pi L)$$

$$\approx \delta_{\mathrm{FV},f_\pi}(M_\pi L)$$

$\Rightarrow$ 10^{-3} correction for physical pion mass and $M_\pi L = 4$

$N\pi$ contribution to ratio R_X

$$\Delta E_n = E_n - M_N$$

$$R_X(t,t') = g_X\left[1 + \sum_{n\le n_{\rm max}} b_{X,n}\left(e^{-\Delta E_n(t-t')} + e^{-\Delta E_n t'}\right) + c_{X,n}e^{-\Delta E_n t}\right]$$

- Non-trivial result of the calculation: The coefficients $b_{X,n}, c_{X,n}$
- For example

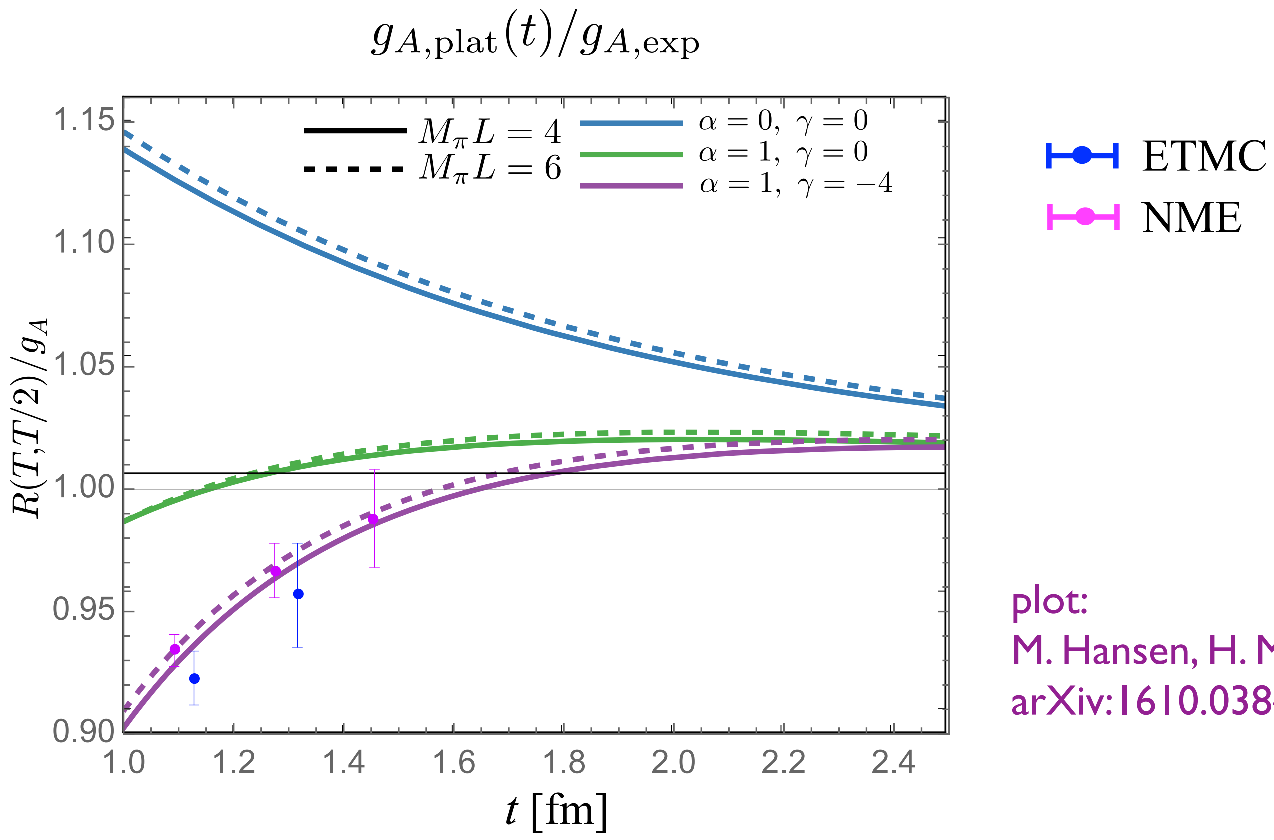
$$c_{X,n} = \frac{m_n}{16(fL)^2 E_{\pi,n} L}\left(1 - \frac{M_{N,\rm ch}}{E_{N,n}}\right) C_{X,n}$$

total $N\pi$ energy

$$C_{A,n} = (\overline{g}_A - 1)^2\,\frac{2}{3}\left(\frac{M_N}{E_{N,n}} - \frac{1}{2}\right) \qquad \overline{g}_A = g_A\frac{E_{N\pi,n} + M_N}{E_{N\pi,n} - M_N}$$

Note:
- vanishes for nucleon/pion at rest (parity!)
- $1/L^3$ suppression of individual coefficients

Comparison with lattice data: axial charge



plot:
M. Hansen, H. Meyer
arXiv:1610.03843

Test: vector current conservation

We assume isospin symmetry $\Rightarrow$ the vector current is conserved

➥ $$C_{3,V_0}(t,t') = g_V C_2(t) \qquad g_V = 1$$

Provides non-trivial test for the MATHEMATICA programs
used to compute the correlation functions

Nucleon interpolating fields in QCD

- Our interest here: Correlators of *nucleon interpolating fields* $N(x)$
  How to map these to ChPT ?

- Starting point: Nucleon interpolating fields in QCD
  We consider
  - local 3-quark operators
  - no derivatives
  - ➥ two independent operators
    Ioffe 1981, Espriu et al 1983

charge conjugation

$$N_1 = (\tilde{q}q)q \qquad q = \begin{pmatrix} u \\ d \end{pmatrix} \qquad \tilde{q} = q^{\mathrm{T}} C\gamma_5 (i\sigma_2)$$
$$N_2 = (\tilde{q}\gamma_5 q)\gamma_5 q$$

antisym sum over color indices suppressed !

- Transformation under chiral symmetry and parity
  Nagata et al 2008

$$N_i = N_{i,R} + N_{i,L} \xrightarrow{R,L} RN_{i,R} + LN_{i,L}$$

$$N_i = N_{i,R} + N_{i,L} \xrightarrow{P} \gamma_0 (N_{i,L} + N_{i,R})$$

Nucleon interpolating fields in ChPT

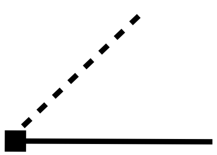
- Map interpolating fields to ChPT and expand

P. Wein et.al. 2011

$$N_i = \alpha_i \left(\Psi + \frac{i}{2f} \pi^a \sigma^a \gamma_5 \Psi + \ldots \right) \quad + \quad \text{higher orders}$$

LO LEC associated with interpolating field

- By construction: Transform as the fields at the quark level
- Note: Same chiral expansion for both operators ($i=1$ and 2), but different LECs α_i
- Expression implies $\Psi\pi$-Vertex



- NLO: two more terms, two more LECs

Smeared interpolating fields

- Often used in Lattice QCD: *Smeared interpolating fields* build from smeared quark fields

$$q_{\rm sm}(x) = \int \mathrm{d}^4y K(x-y) q(y) \quad \Rightarrow \quad \begin{aligned} N_{1,\rm sm} &= (\tilde{q}_{\rm sm} q_{\rm sm}) q_{\rm sm} \\ N_{2,\rm sm} &= (\tilde{q}_{\rm sm} \gamma_5 q_{\rm sm}) \gamma_5 q_{\rm sm} \end{aligned}$$

- The gauge covariant kernel K
  - is essentially zero for $|x-y| > R_{\rm smear}$ (``*smearing radius*")
  - contains a delta function in time for *Gaussian smearing* Gasket 1989, Alexandrou et. al. 1991
  - is truly 4-dimensional for the gradient flow Lüscher 2013
  - is diagonal in spinor space

If $R_{\rm smear} \ll \dfrac{1}{M_\pi}$ $\Rightarrow$ Smeared fields map to the same point-like fields as their unsmeared counterparts

Difference in the LECs only