
Lattice QCD Results on Moments of Nucleon Parton Distribution Functions and Generalized Form Factors

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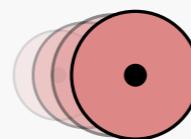
Outline

Moments of PDFs

- Lower moments of PDFs from the lattice
 - Axial and tensor charge
 - Intrinsic quark spin contribution to nucleon spin
- Moments of PDFs
 - Momentum fraction
 - Helicity and transversity
- Momentum dependence
 - Generalized form factors

Unpolarised

$$\mathcal{O}_V^{\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi}\gamma^{\{\mu}iD^{\mu_1}iD^{\mu_2}\dots iD^{\mu_n\}}\psi$$



Helicity

$$\mathcal{O}_A^{\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi}\gamma_5\gamma^{\{\mu}iD^{\mu_1}iD^{\mu_2}\dots iD^{\mu_n\}}\psi$$



Transverse

$$\mathcal{O}_T^{\nu\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi}\sigma^\nu\gamma^{\{\mu}iD^{\mu_1}iD^{\mu_2}\dots iD^{\mu_n\}}\psi$$



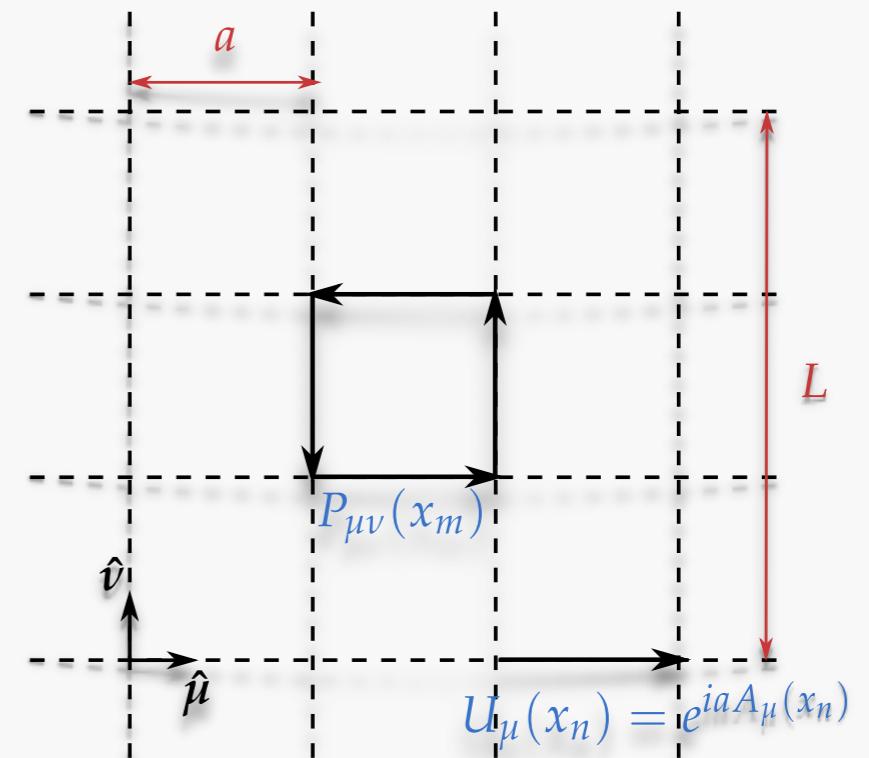
Lattice QCD — ab initio simulation of QCD

Numerical solution of Quantum Chromodynamics

- Direct simulation, starting from the QCD Lagrangian

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D[\mathbf{U}] \mathcal{O}[\mathbf{M}^{-1}] e^{-S_g[\mathbf{U}] + \ln \det \mathbf{M}}$$

- Path integral formulation allows for Markov Chain Monte-Carlo simulation
- Integrate-out fermion fields: Need inverse: \mathbf{M}^{-1}
- Sample representative sets of gluon fields \mathbf{U}



Lattice QCD — ab initio simulation of QCD

Freedom in choice of:

- quark masses (**heavier is cheaper**)
- lattice spacing a (**larger is cheaper**)
- lattice volume $L^3 \times T$ (**smaller is cheaper**)

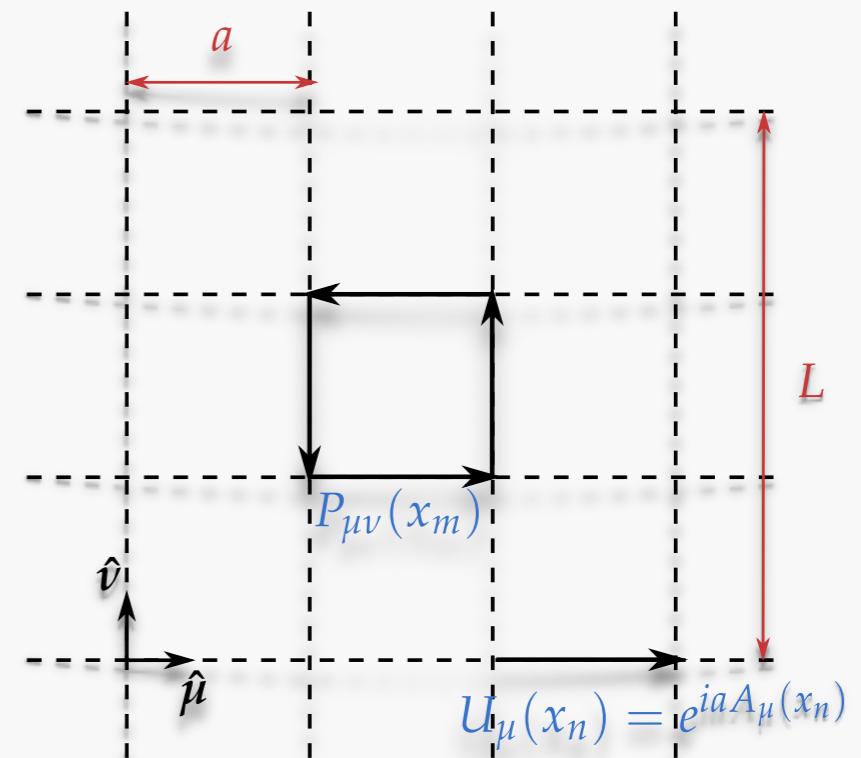
Choice of discretisation scheme

e.g. **Clover, Twisted Mass, Staggered, Overlap, Domain Wall**

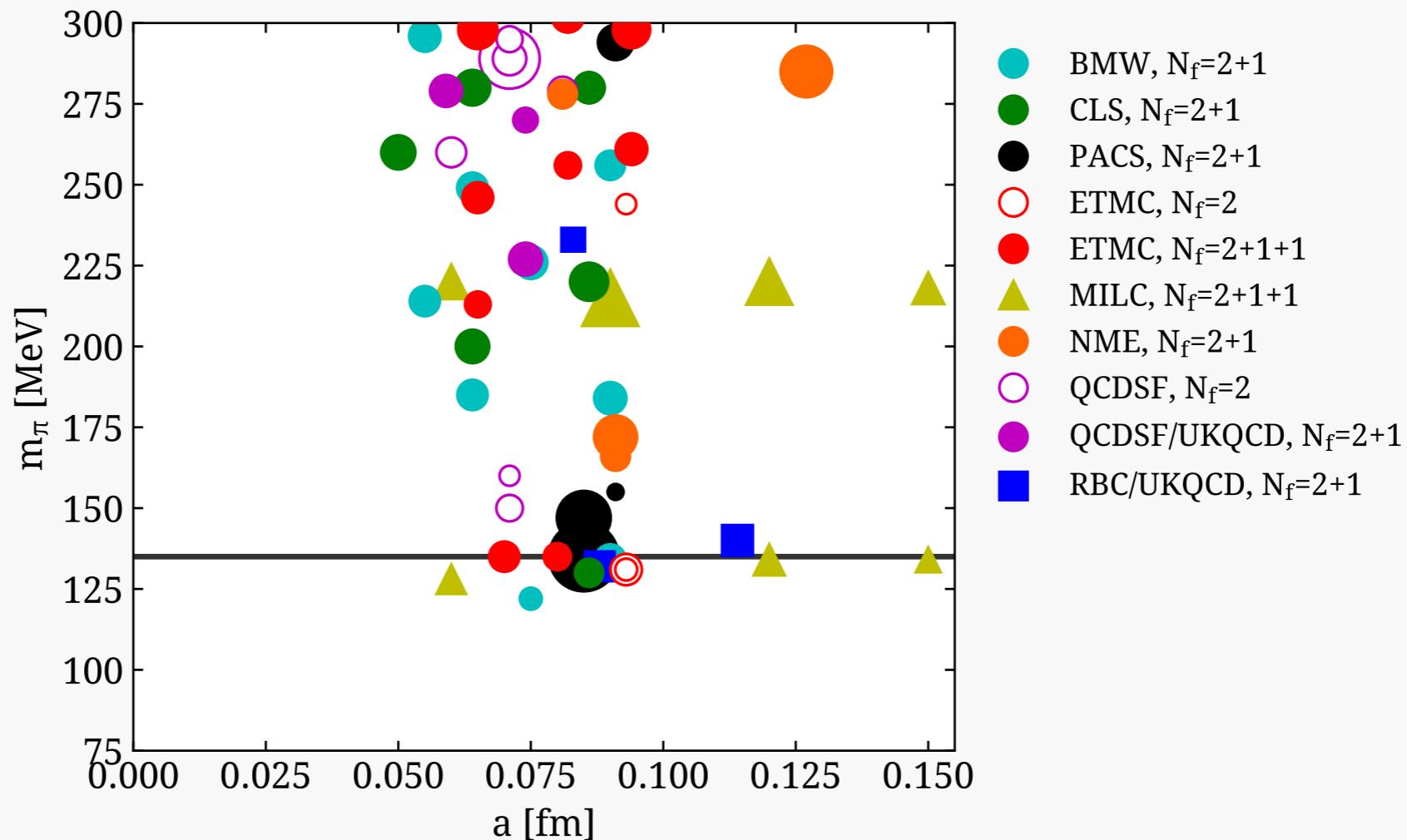
Trade – offs and advantages for each differ

Eventually, all schemes must agree:

- At the continuum limit: $a \rightarrow 0$
- At infinite volume limit $L \rightarrow \infty$
- At physical quark mass



Simulation landscape



Selected lattice simulation points used for hadron structure

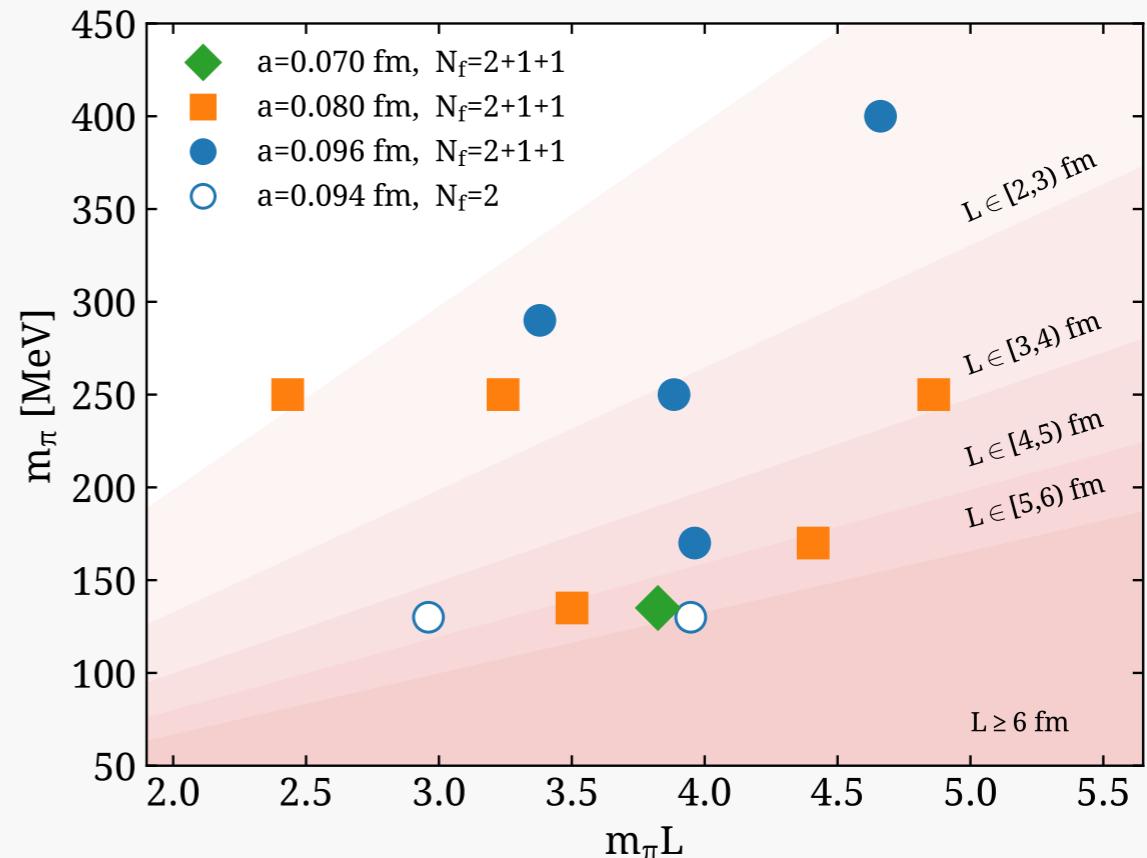
- Multiple collaborations simulating at physical pion mass
- Size of points indicates $m_\pi L$

Twisted Mass QCD

$$S_{tm}^\ell = \sum_x \bar{\chi}_\ell(x) \left[D_W(U) + \frac{i}{4} c_{sw} \sigma^{\mu\nu} \mathcal{F}^{\mu\nu}(U) + m + i\mu_\ell \tau^3 \gamma^5 \right] \chi_\ell(x)$$

Formulation particularly attractive for nucleon structure

- Tune to “maximal twist”: tune Wilson mass (m) to its critical value (m_{crit})
- $\mathcal{O}(a)$ improved operators without requiring further operator improvement
- Several ensembles at physical quark mass
- Generation of additional ensembles ongoing



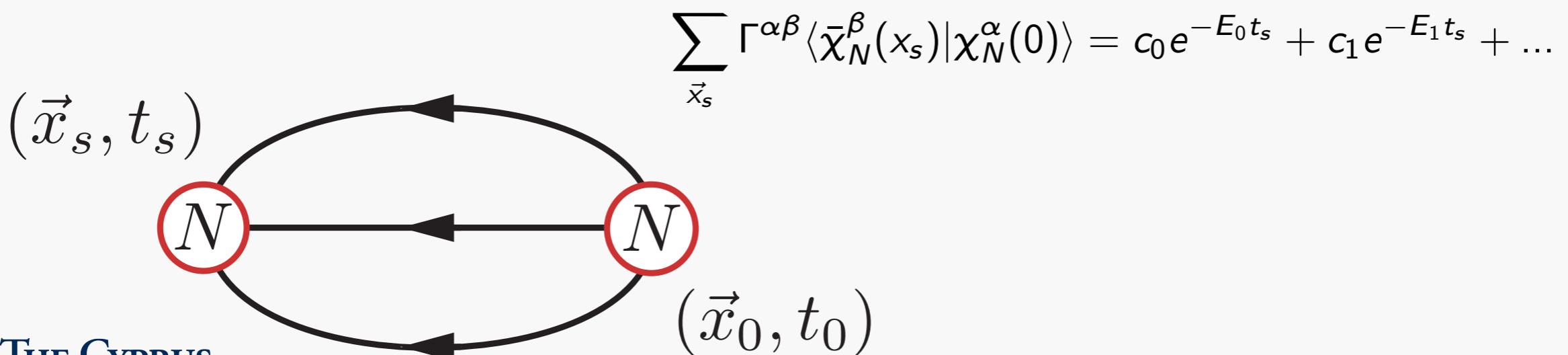
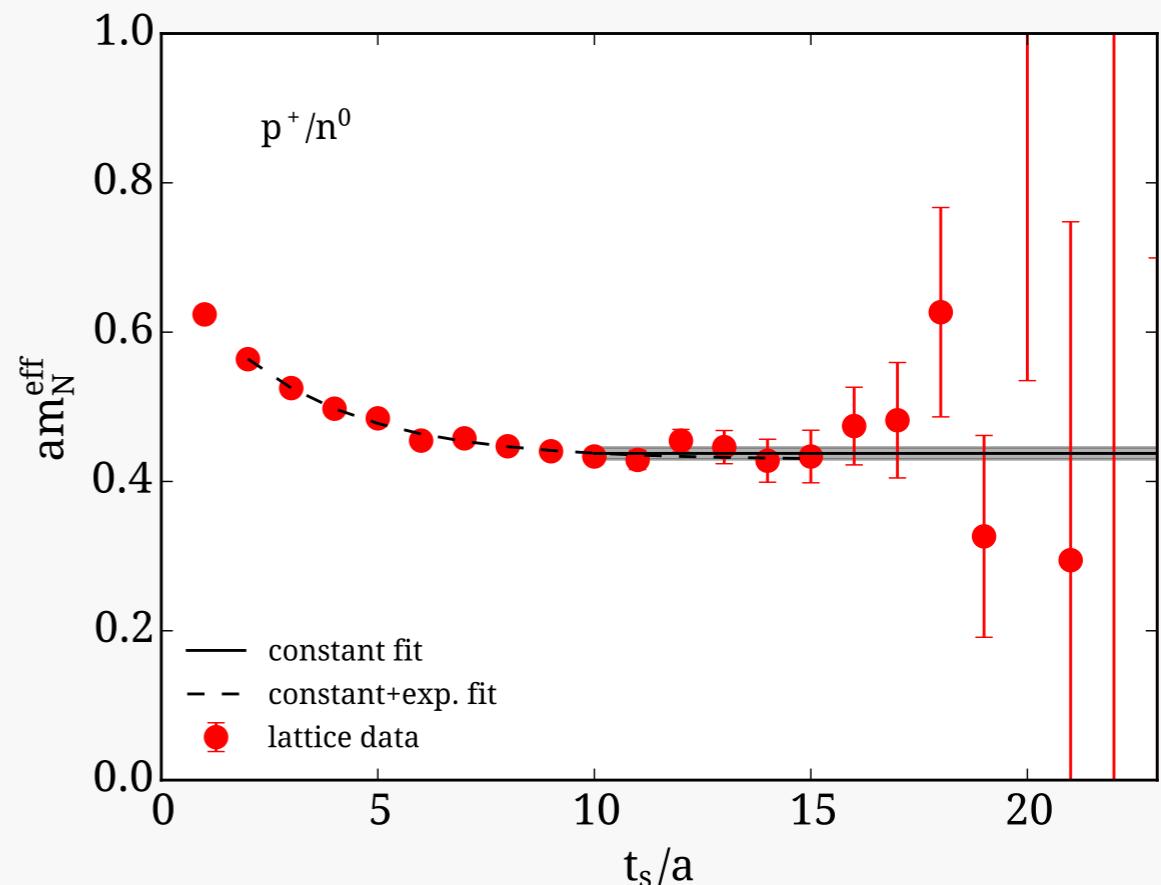
Nucleon structure on the lattice

Two-point correlation functions

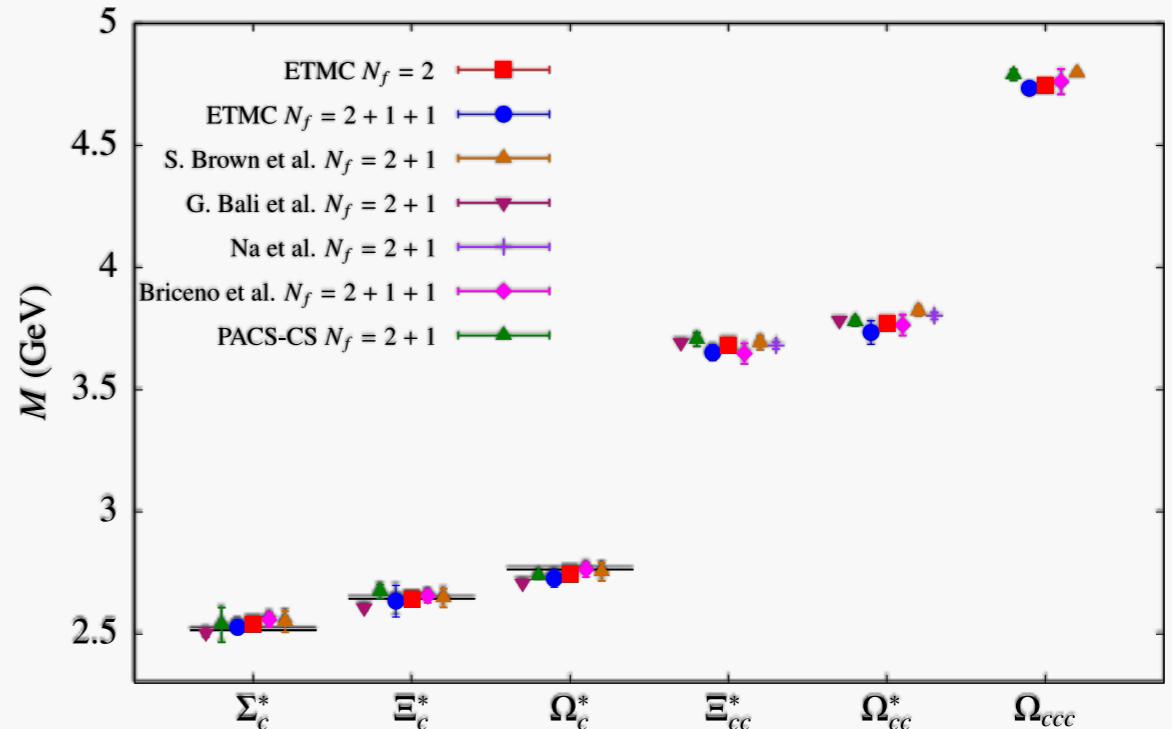
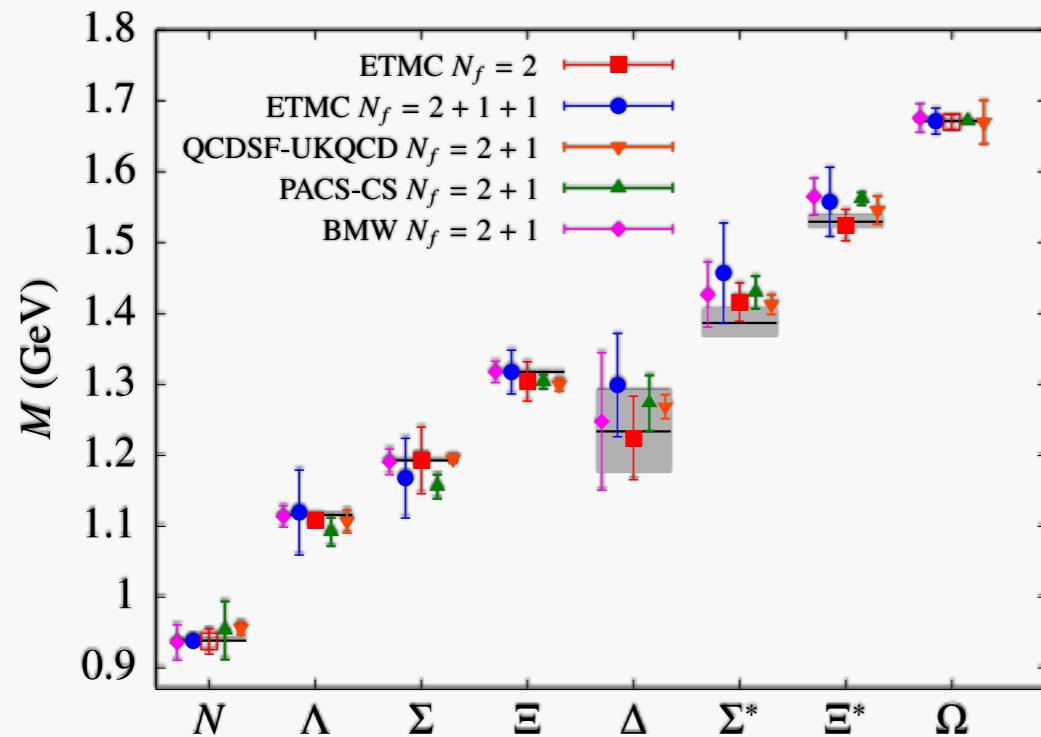
- Statistical error: $N^{-1/2}$ with Monte Carlo samples
- Correlation functions exponentially decay with time-separation

Systematic uncertainties

- Extrapolations: a, L, m_π
- Contamination from higher energy states



Baryon spectrum



Summary plots from arXiv:1704.02647

Reproduction of light baryon masses

- Agreement between lattice discretisations
- Reproduction of experiment

Prediction of yet to be observed baryons

- Confidence through agreement between lattice schemes

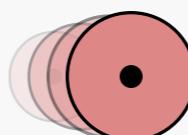
Nucleon structure on the lattice

On the lattice, moments of parton distribution functions are readily accessible as matrix elements of local operators

Unpolarised

$$\mathcal{O}_V^{\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi} \gamma^\mu iD^{\mu_1} iD^{\mu_2} \dots iD^{\mu_n} \psi$$

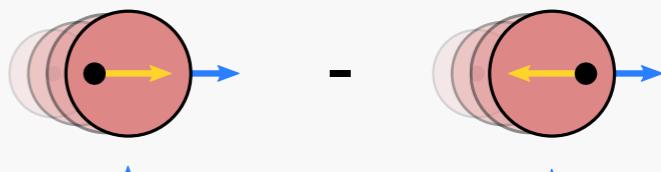
$$\langle 1 \rangle_{u-d} = g_V, \quad \langle x \rangle_{u-d}, \quad \dots$$



Helicity

$$\mathcal{O}_A^{\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi} \gamma_5 \gamma^\mu iD^{\mu_1} iD^{\mu_2} \dots iD^{\mu_n} \psi$$

$$\langle 1 \rangle_{\Delta u - \Delta d} = g_A, \quad \langle x \rangle_{\Delta u - \Delta d}, \quad \dots$$



Transverse

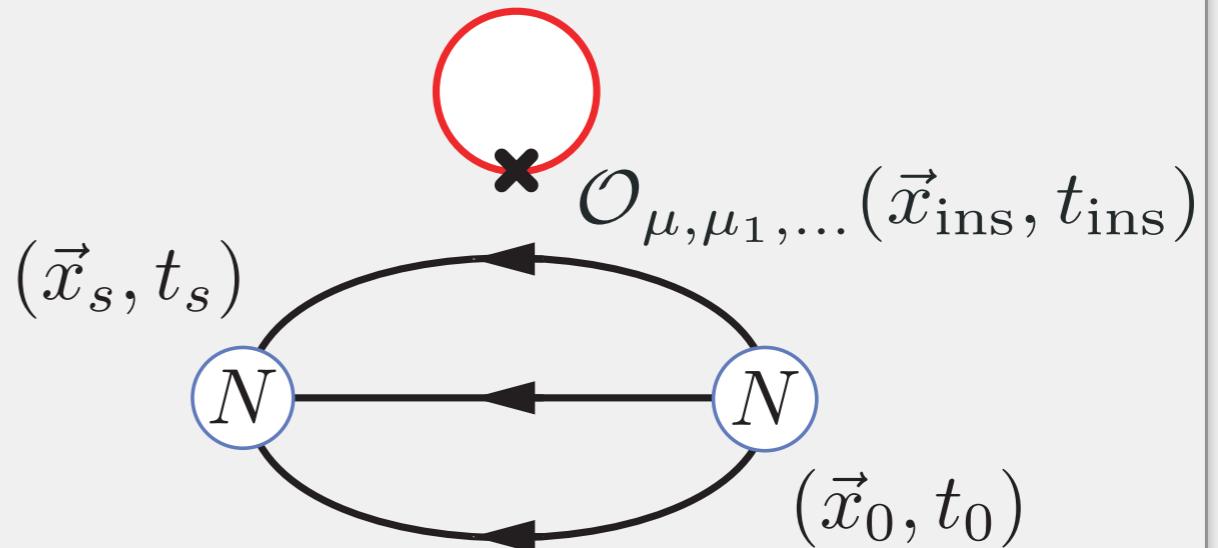
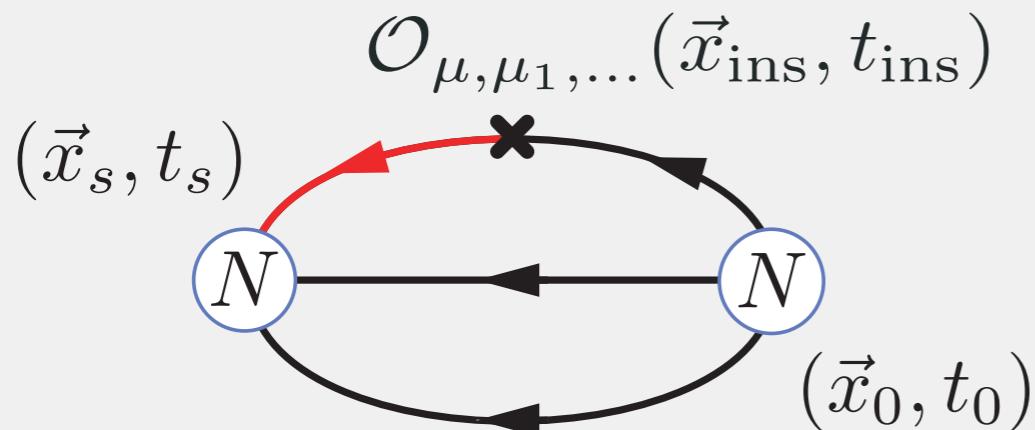
$$\mathcal{O}_T^{\nu\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi} \sigma^\nu \gamma^\mu iD^{\mu_1} iD^{\mu_2} \dots iD^{\mu_n} \psi$$

$$\langle 1 \rangle_{\delta u - \delta d} = g_T, \quad \langle x \rangle_{\delta u - \delta d}, \quad \dots$$



Lattice evaluation of matrix elements

$$G_\mu(\Gamma; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} \Gamma^{\alpha\beta} \langle \bar{\chi}_N^\beta(\vec{x}_s; t_s) | \mathcal{O}^\mu(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_N^\alpha(\vec{0}; 0) \rangle$$



Analyses for identifying excited state contributions

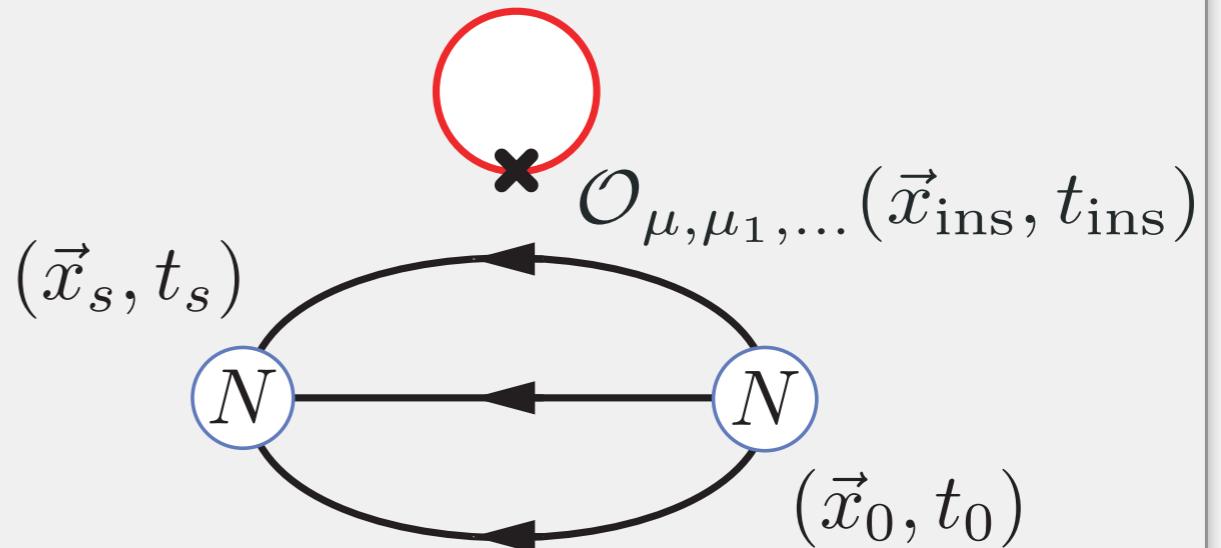
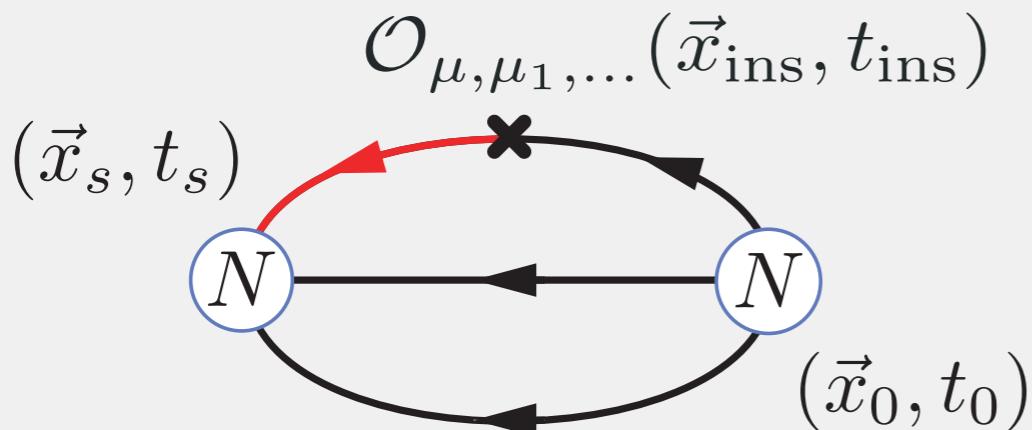
- **Plateau:**

$$R(t_s, t_{\text{ins}}, t_0) \xrightarrow[t_{\text{ins}} - t_0 \rightarrow \infty]{t_s - t_{\text{ins}} \rightarrow \infty} \mathcal{M}[1 + \mathcal{O}(e^{-\Delta(t_{\text{ins}} - t_0)}, e^{-\Delta'(t_s - t_{\text{ins}})})]$$

fit to constant w.r.t. t_{ins} for multiple values of t_s

Lattice evaluation of matrix elements

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Analyses for identifying excited state contributions

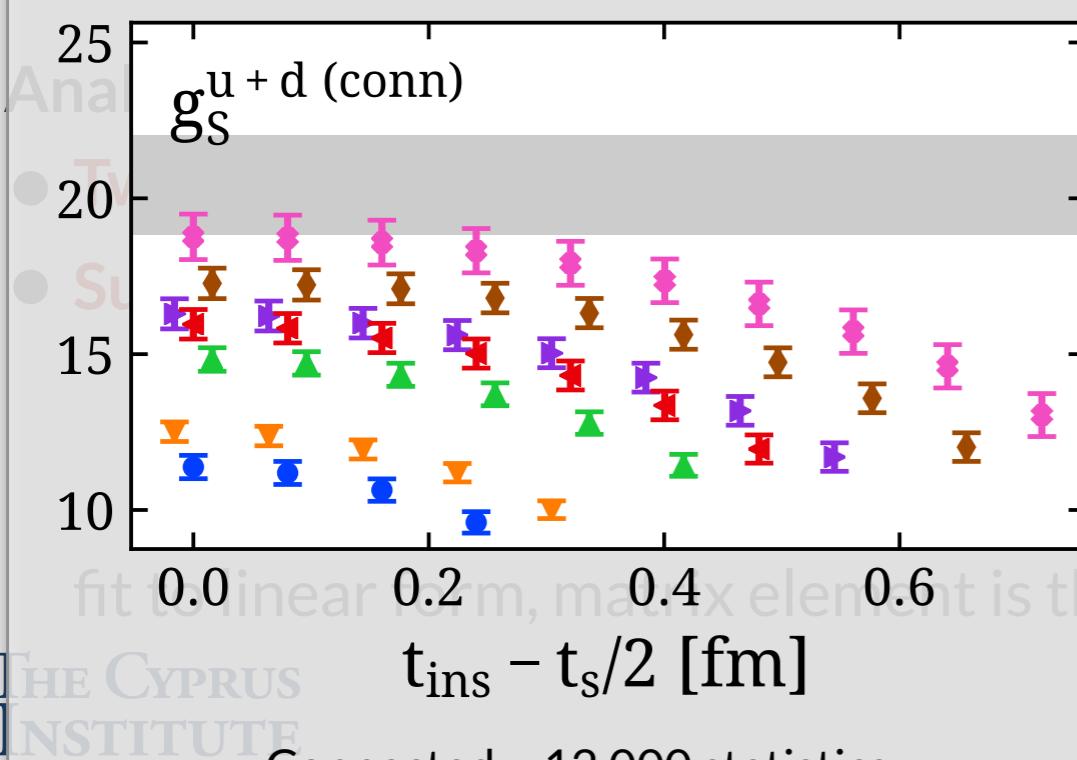
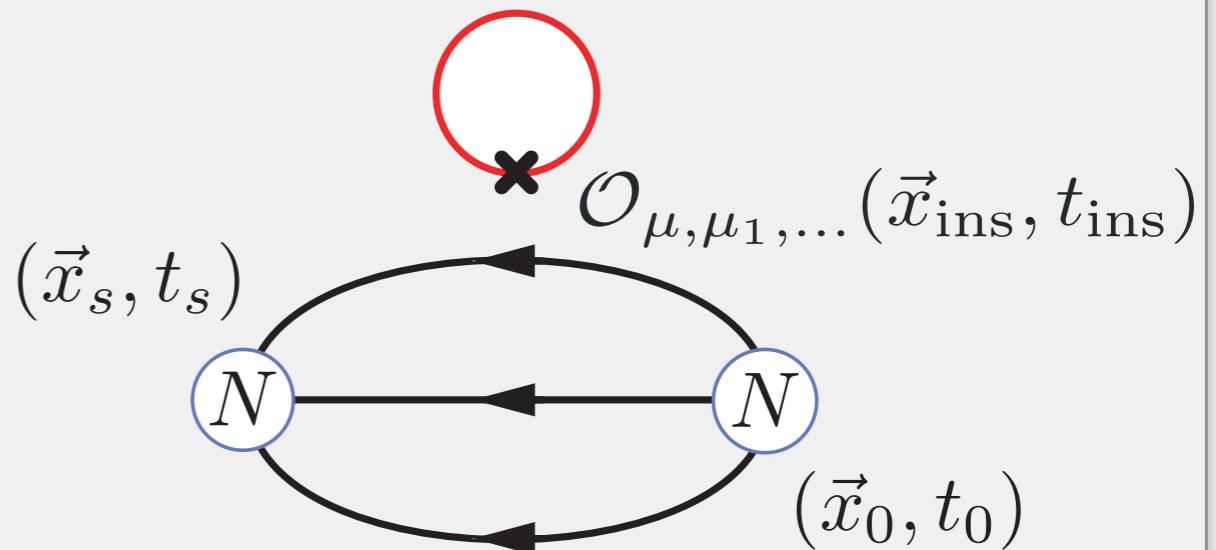
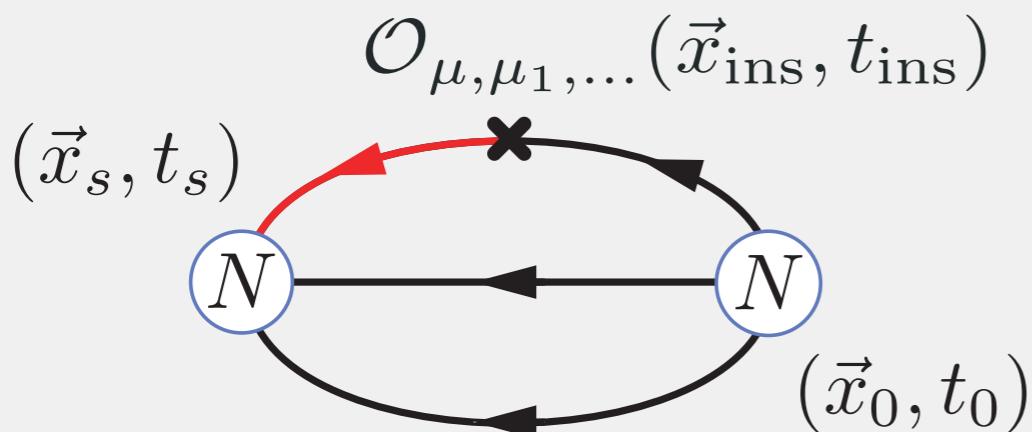
- **Two-state fit:** Fit, two- and three-point simultaneously, including first excited state
- **Sum over t_{ins} :**

$$\sum_{t_{\text{ins}}} R(t_s, t_{\text{ins}}, t_0) \xrightarrow{t_s - t_0 \rightarrow \infty} \text{Const.} + \mathcal{M}(t_s - t_0) + \mathcal{O}(t_s e^{-\Delta t_s})$$

fit to linear form, matrix element is the slope.

Lattice evaluation of matrix elements

$$G_\mu(\Gamma; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} \Gamma^{\alpha\beta} \langle \bar{\chi}_N^\beta(\vec{x}_s; t_s) | \mathcal{O}^\mu(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_N^\alpha(0; 0) \rangle$$



contributions

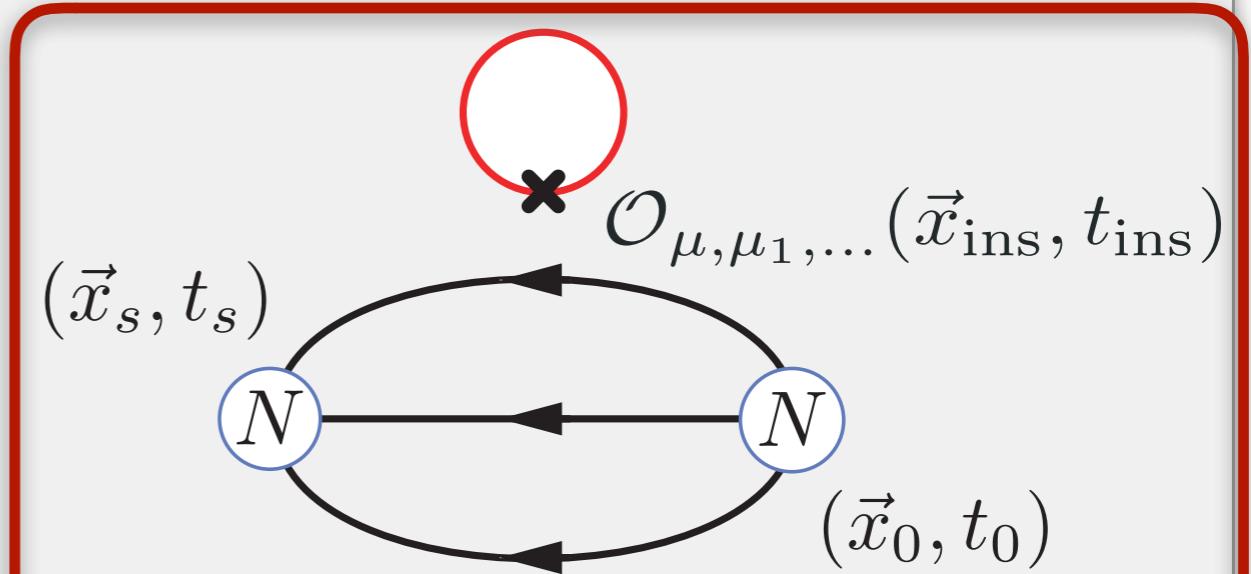
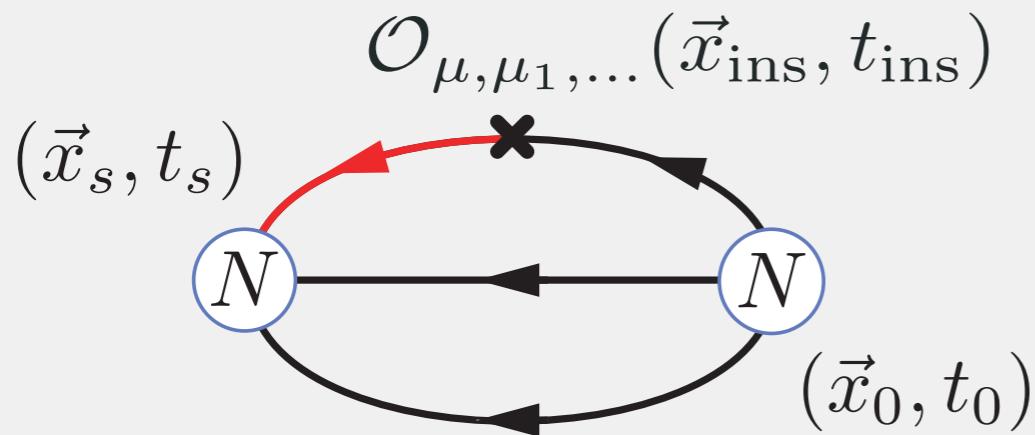
simultaneously, including first excited state

Const. + $\mathcal{M}(t_s - t_0) + \mathcal{O}(t_s e^{-\Delta t_s})$

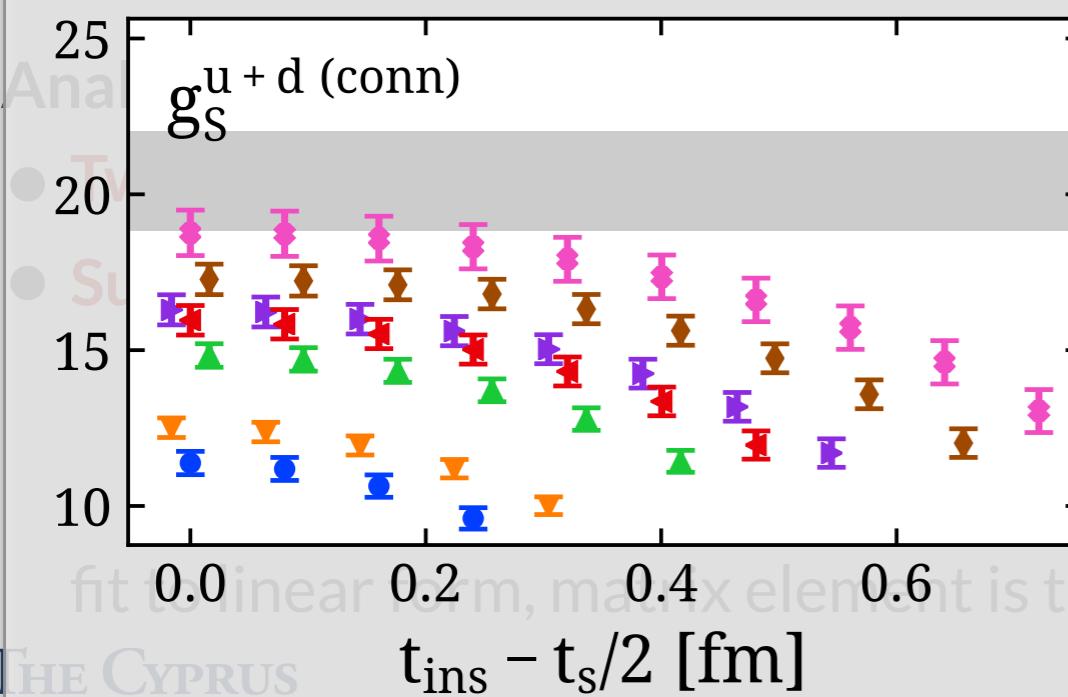
slope.

Lattice evaluation of matrix elements

$$G_\mu(\Gamma; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} \Gamma^{\alpha\beta} \langle \bar{\chi}_N^\beta(\vec{x}_s; t_s) | \mathcal{O}^\mu(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_N^\alpha(0; 0) \rangle$$



“Disconnected” contributions – estimate stochastically



contributions

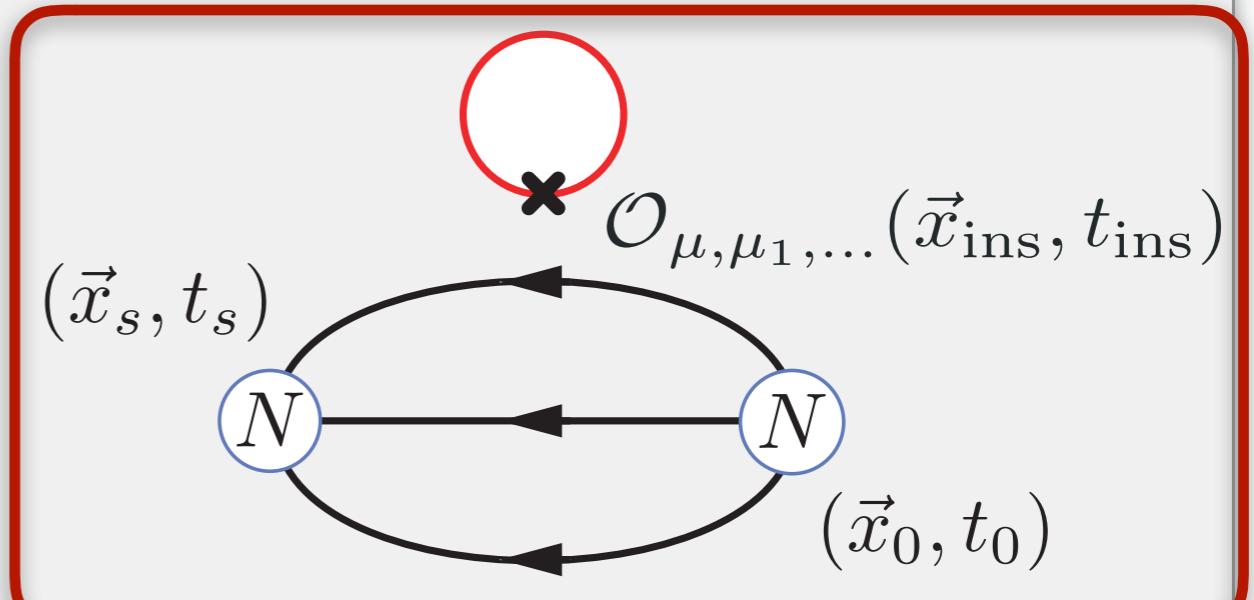
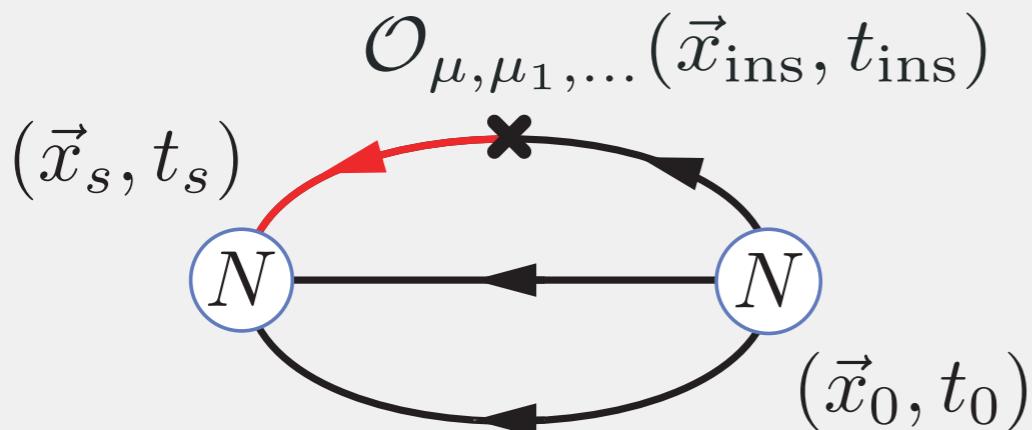
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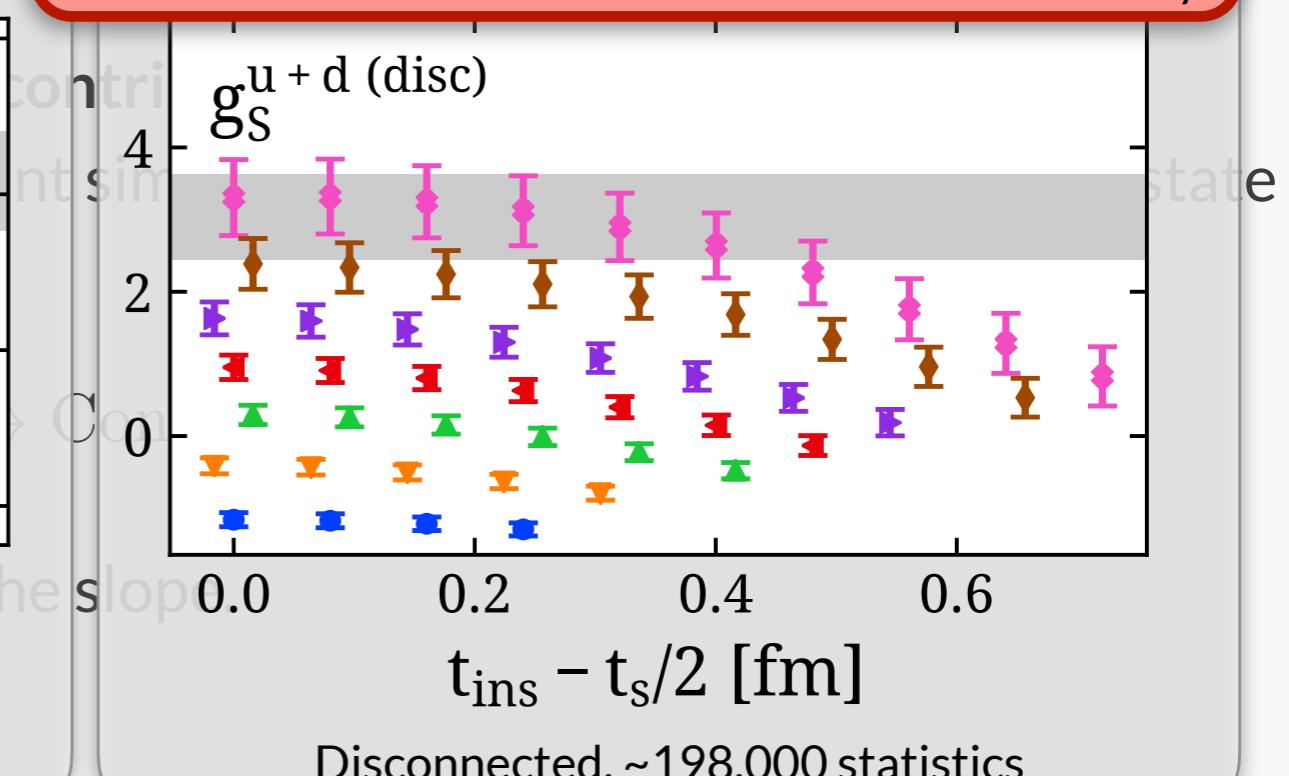
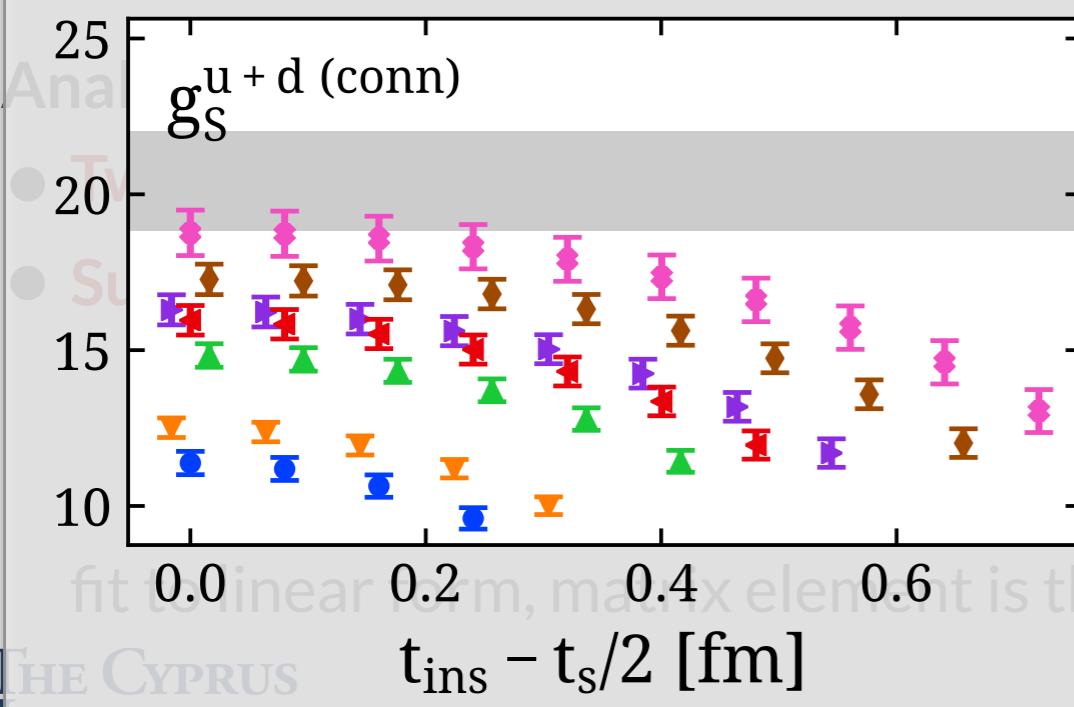
slope.

Lattice evaluation of matrix elements

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“Disconnected” contributions – estimate stochastically

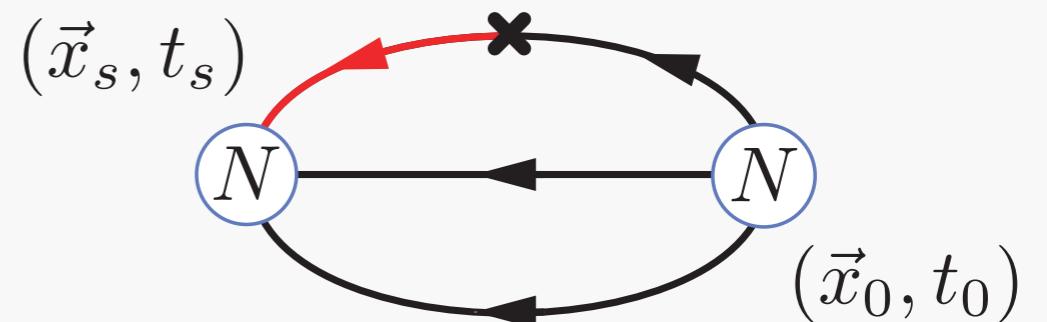


Axial Matrix Elements

$$\mathcal{O}^A = \bar{u}\gamma_5\gamma_k u - \bar{d}\gamma_5\gamma_k d$$

Axial charge:

- Well known from β -decay
- Readily accessible on the lattice
- Benchmark quantity in lattice QCD

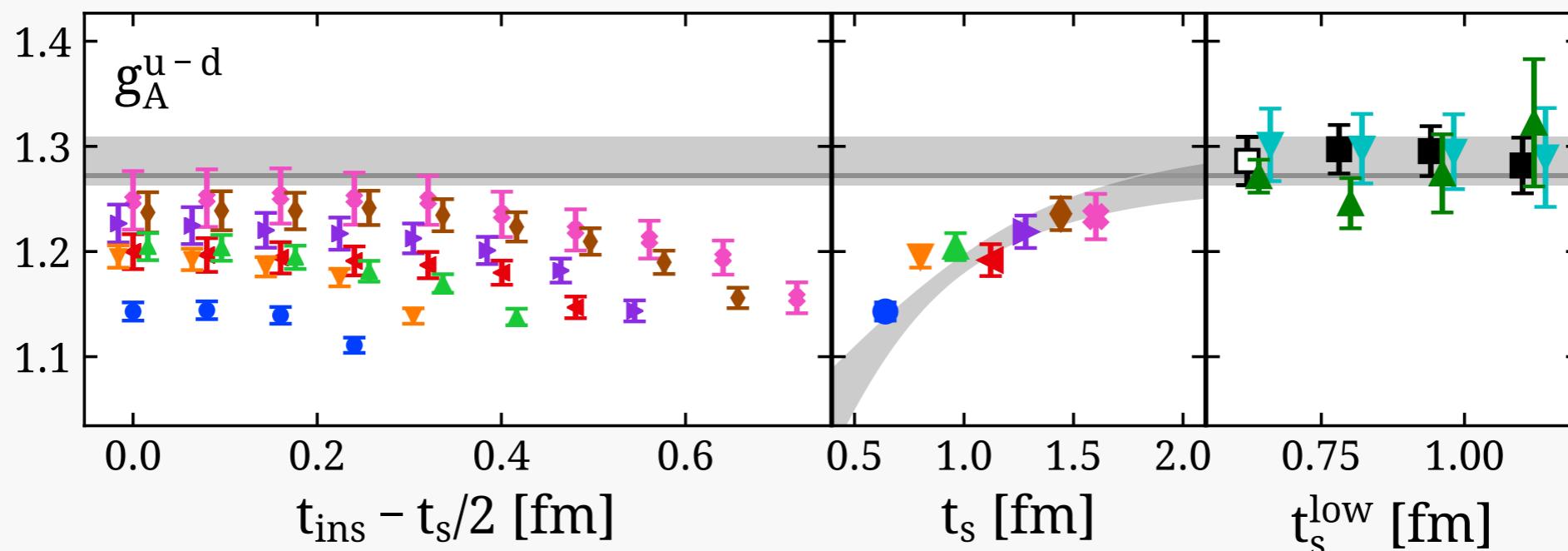
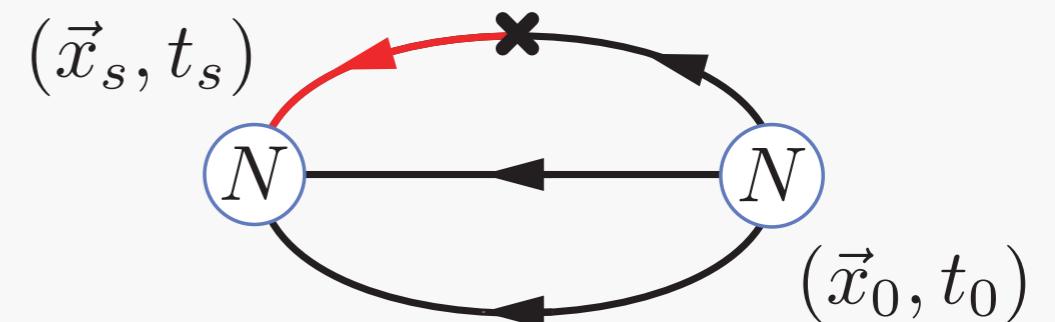


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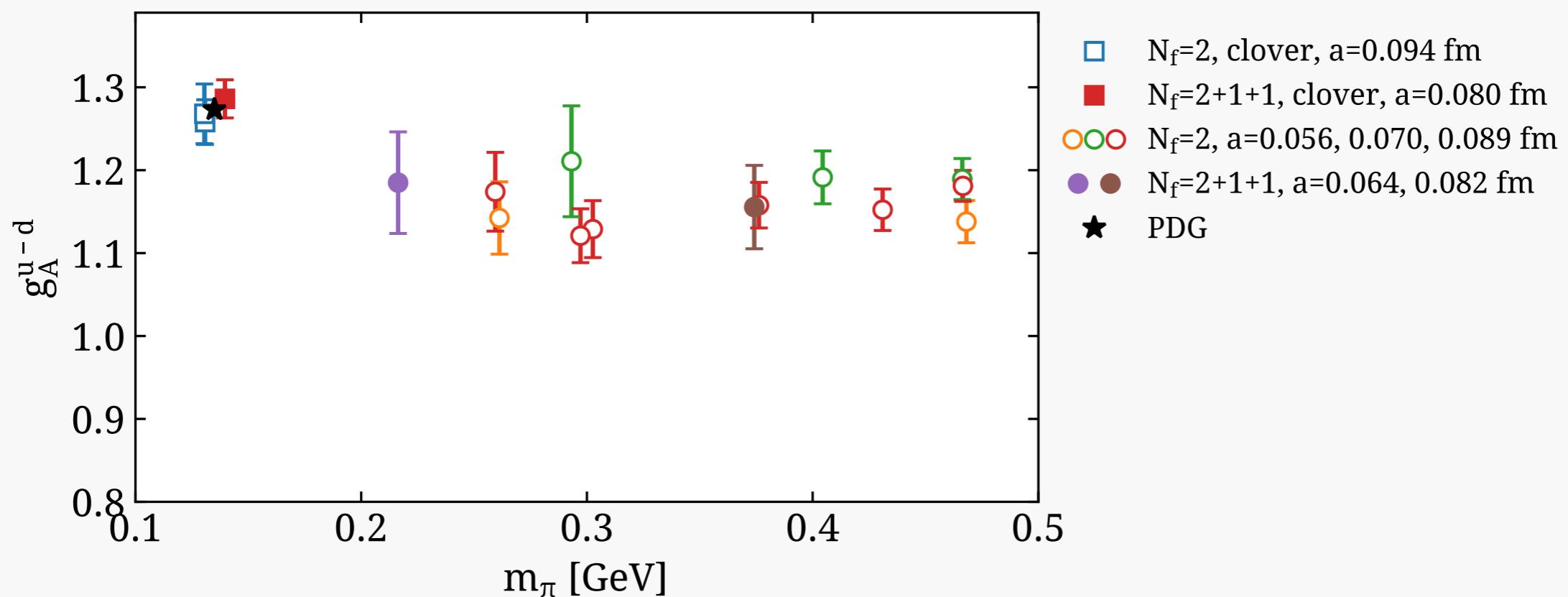
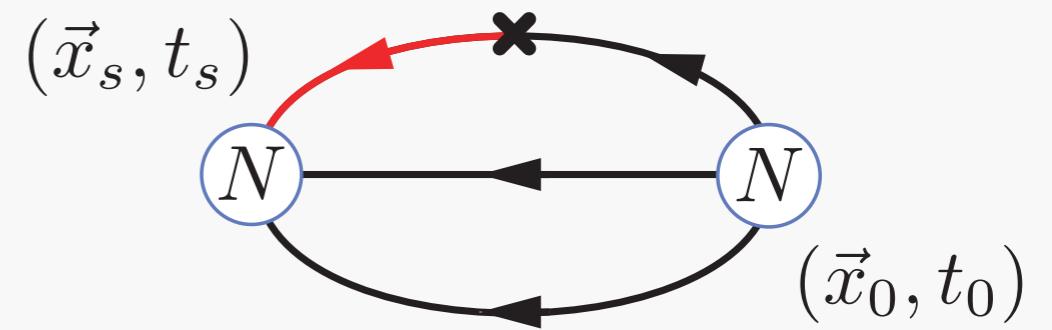
Treatment of excited states
Asymptotic value consistent between methods

Axial Matrix Elements

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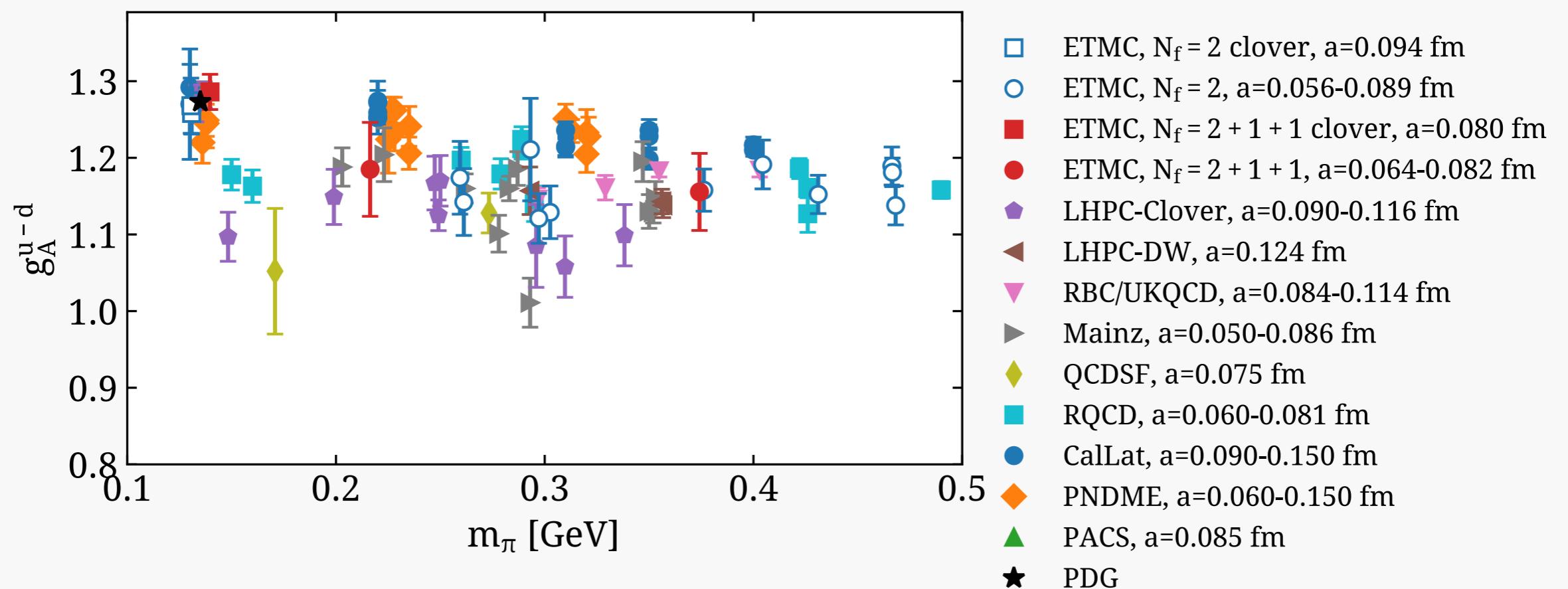
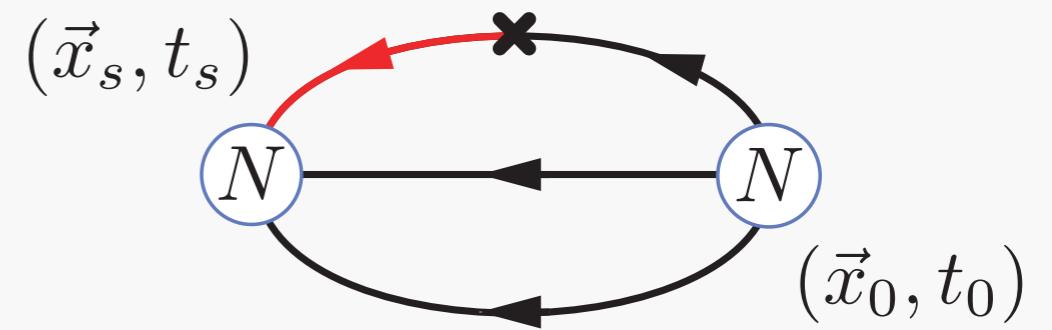


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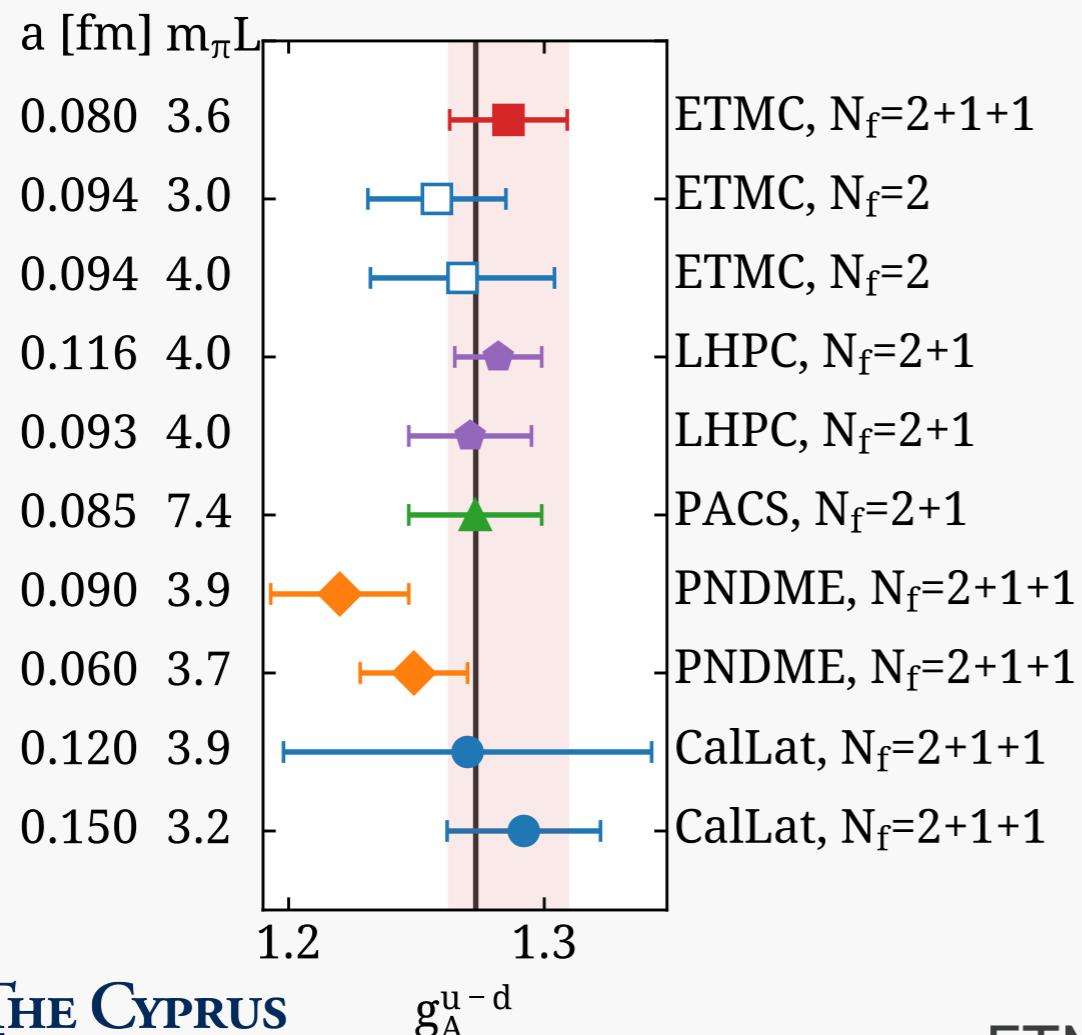
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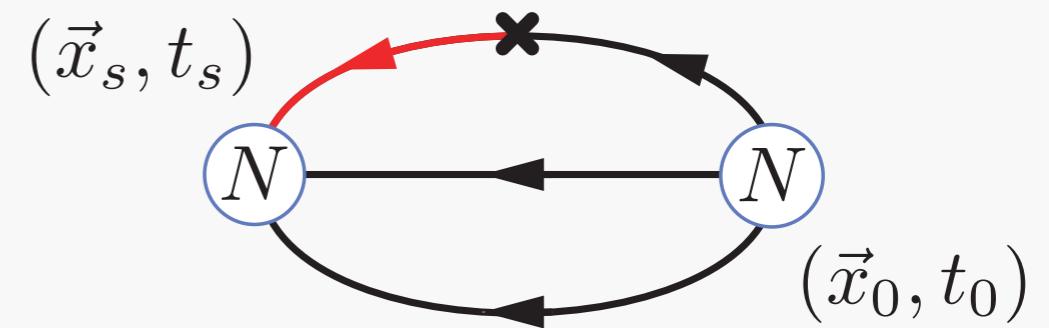
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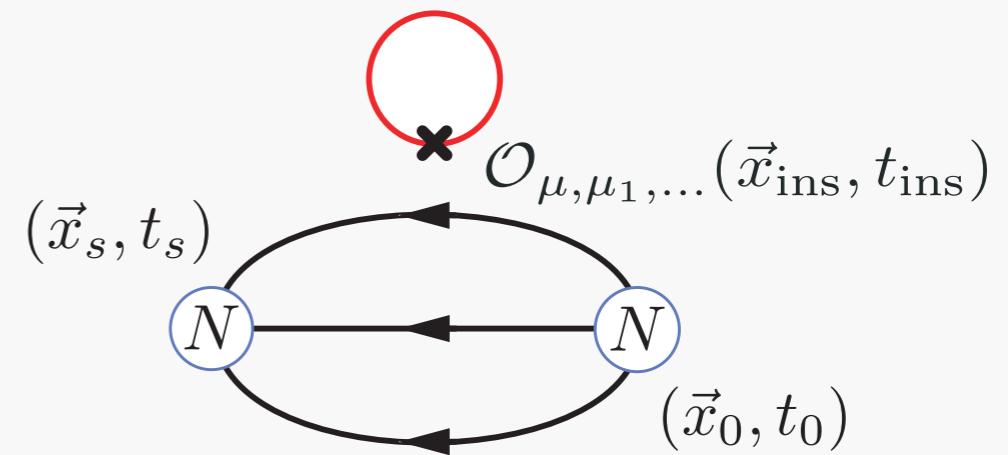
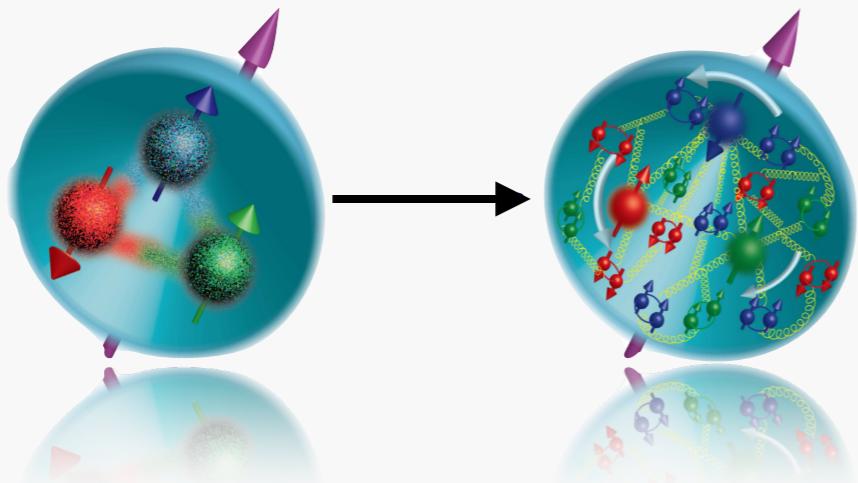
Lattice status

- Range of lattice actions
- Range of volumes and lattice spacings
- Agreement with experiment:
 - Physical point simulations
 - Careful analysis of ground state dominance

Nucleon spin

Quark intrinsic spin contributions to nucleon spin

$$\frac{1}{2} \Delta \Sigma = \frac{1}{2} \sum_{q=u,d,s,\dots} g_A^q$$



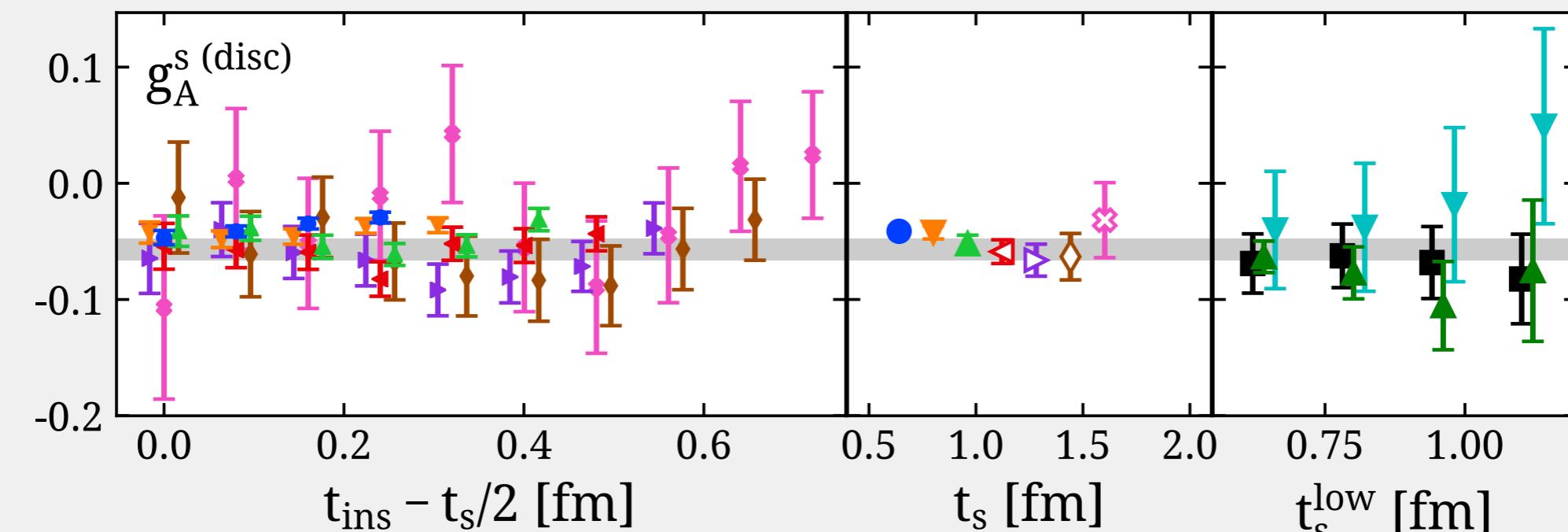
Quark intrinsic spin contributions to nucleon spin

- Need linear combination of isovector ($u-d$) and isoscalar ($u+d$) contributions for individual up- and down-quarks
- Strange quark contribution is sea-quark contribution only (disconnected diagrams)
- Need $O(10) - O(100)$ times more statistics

Nucleon spin

Quark intrinsic spin contributions to nucleon spin

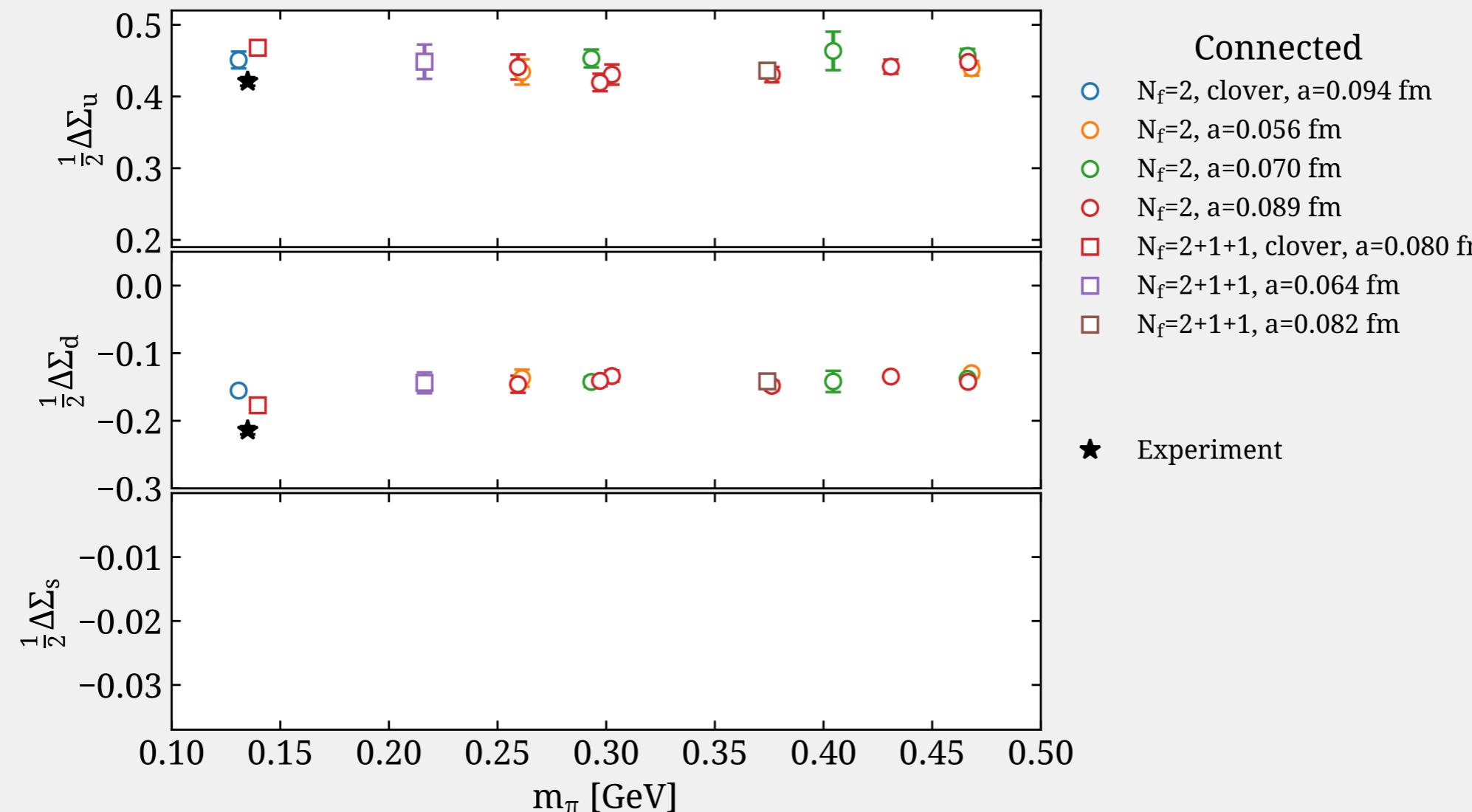
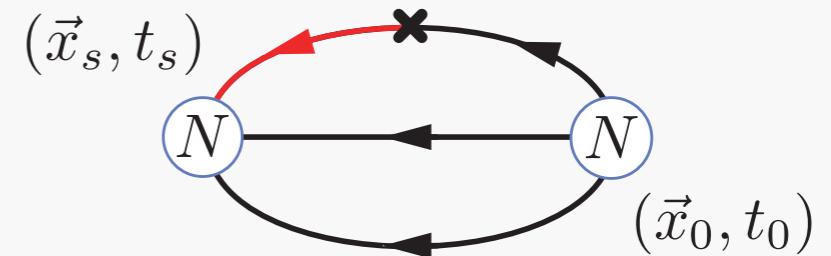
$$\frac{1}{2} \Delta \Sigma = \frac{1}{2} \sum_{q=u,d,s,\dots} g_A^q$$



Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

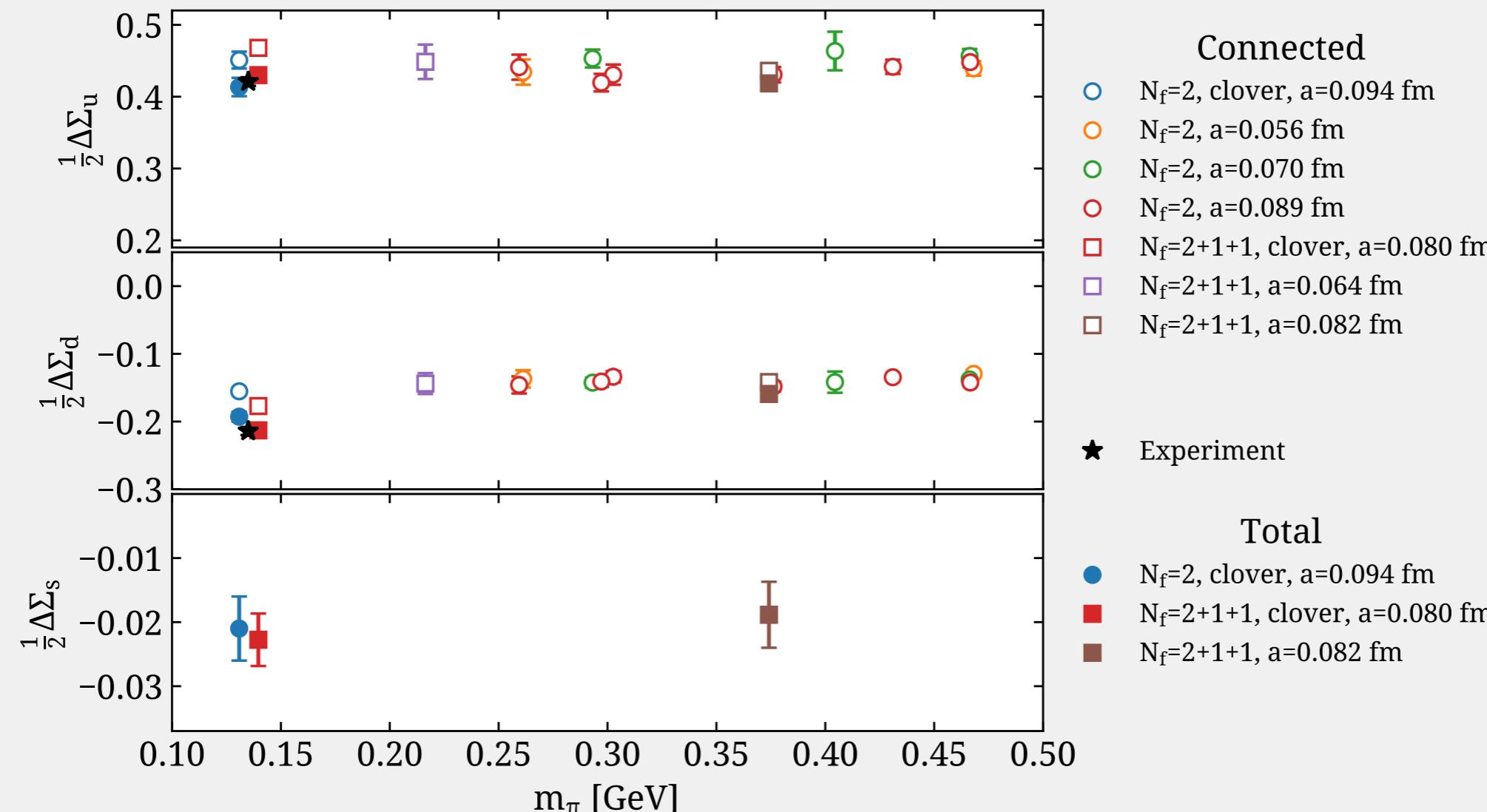
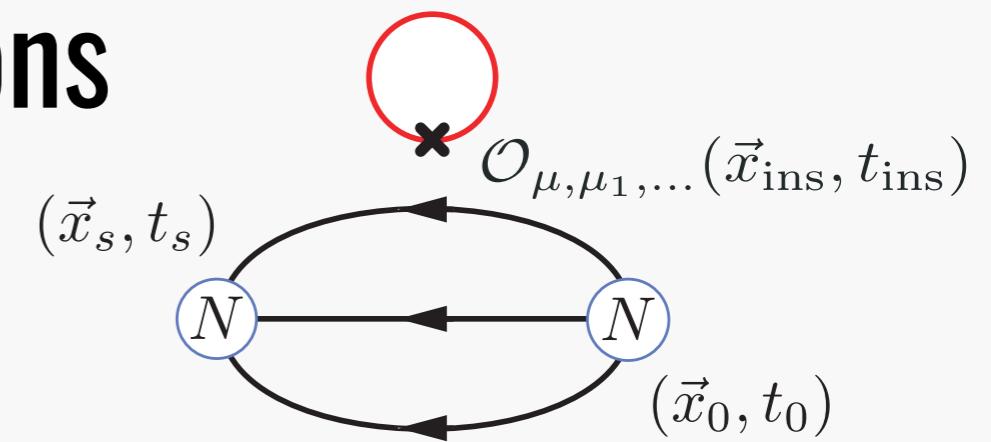
- Mild cut-off effects
- Strange and down-quark contributions negative



Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

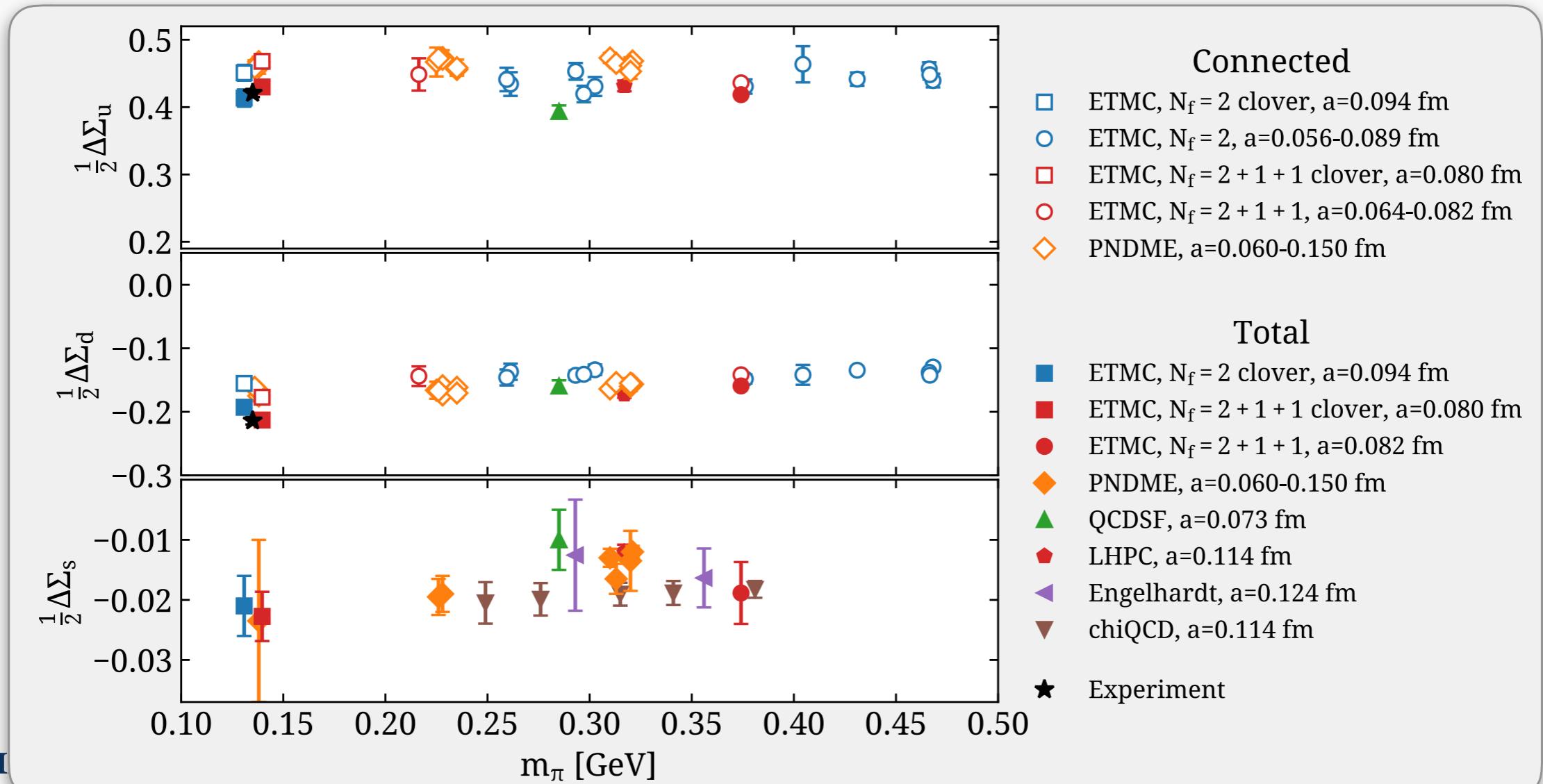
- Mild cut-off effects
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- Disconnected contributions: agreement with experiment



Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

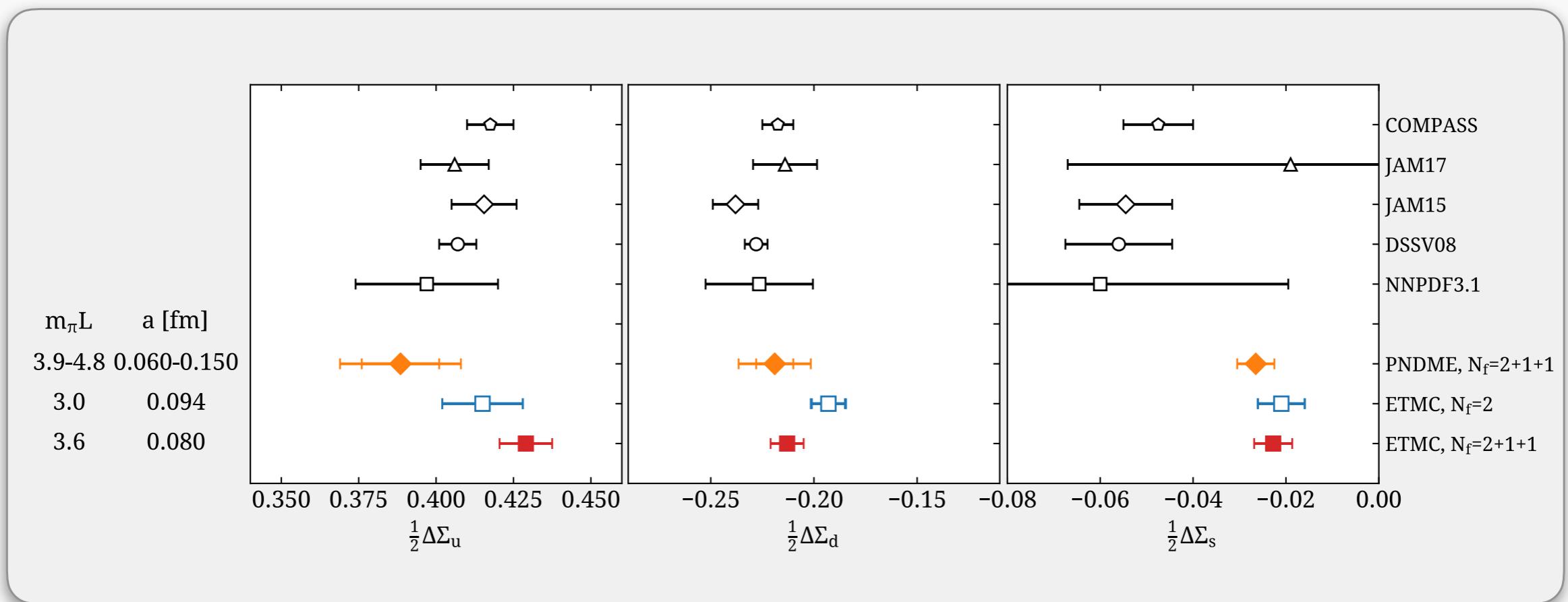
- Mild cut-off effects
- Strange and down-quark contributions negative
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Quark intrinsic spin contributions

Quark intrinsic spin contributions to nucleon spin

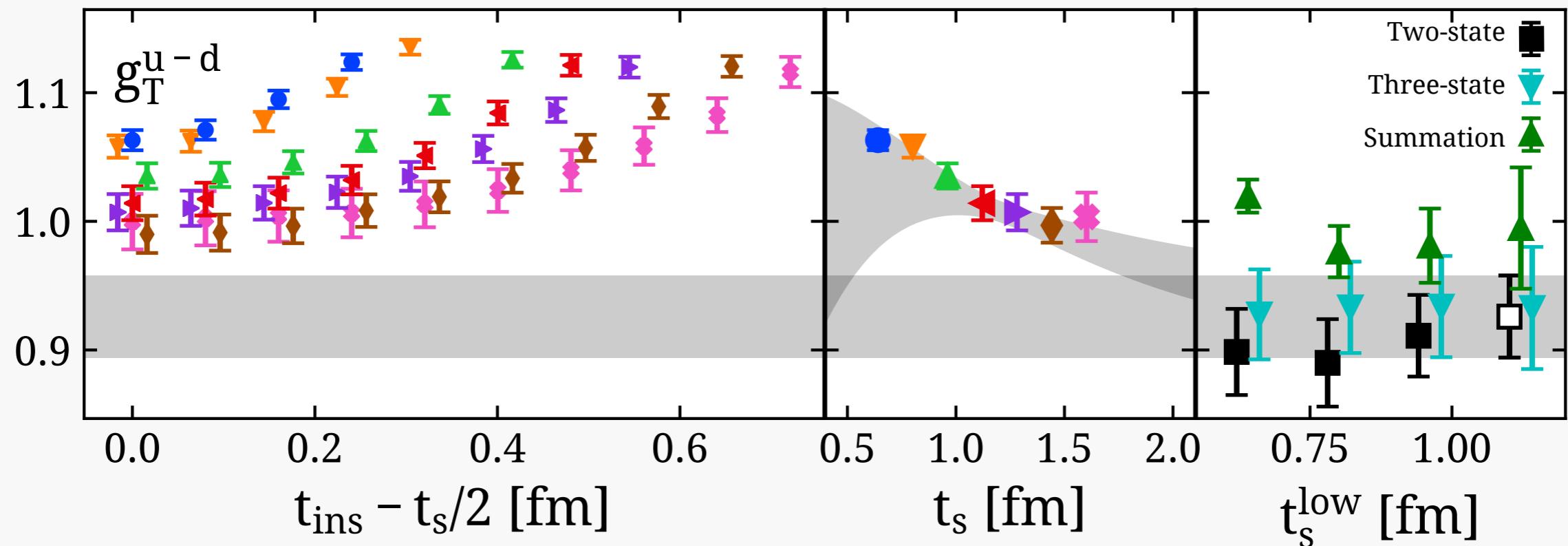
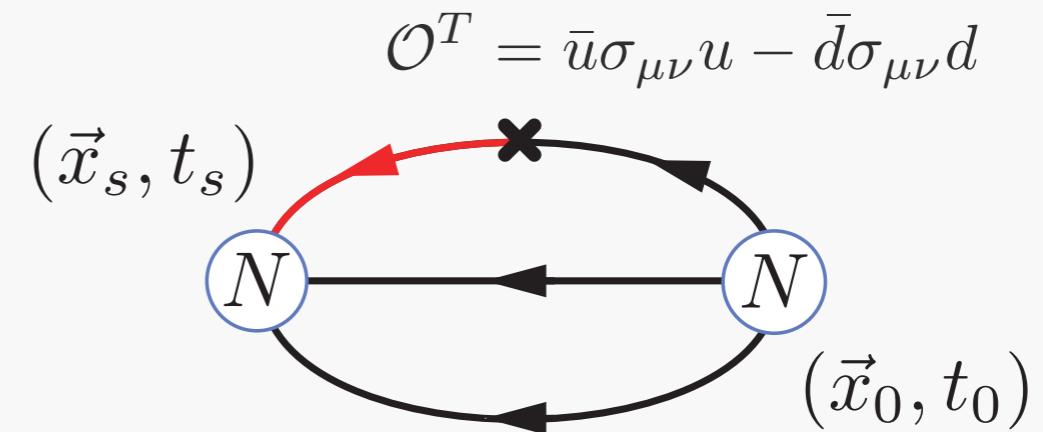
- Individual up-, down-, and strange-quark intrinsic spin contributions to nucleon spin
- Lattice comparison to experiment



Tensor charge

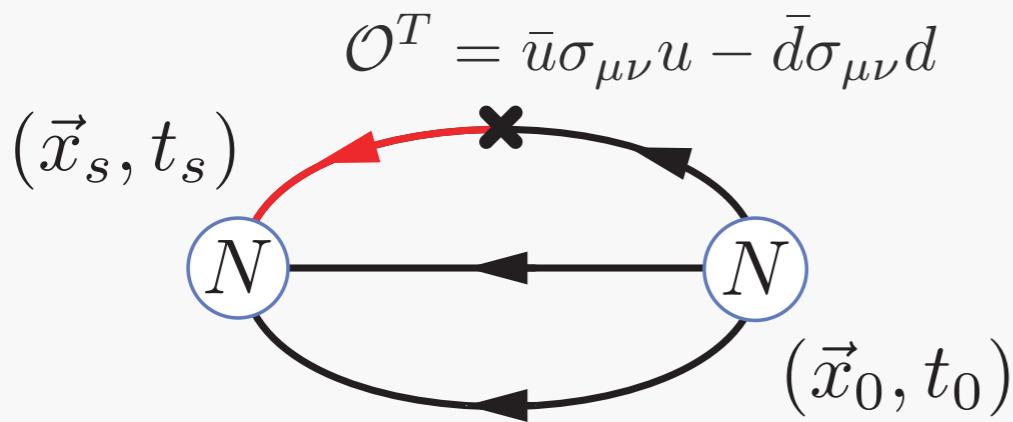
Isovector tensor charge

- Slower convergence to ground state compared to g_A

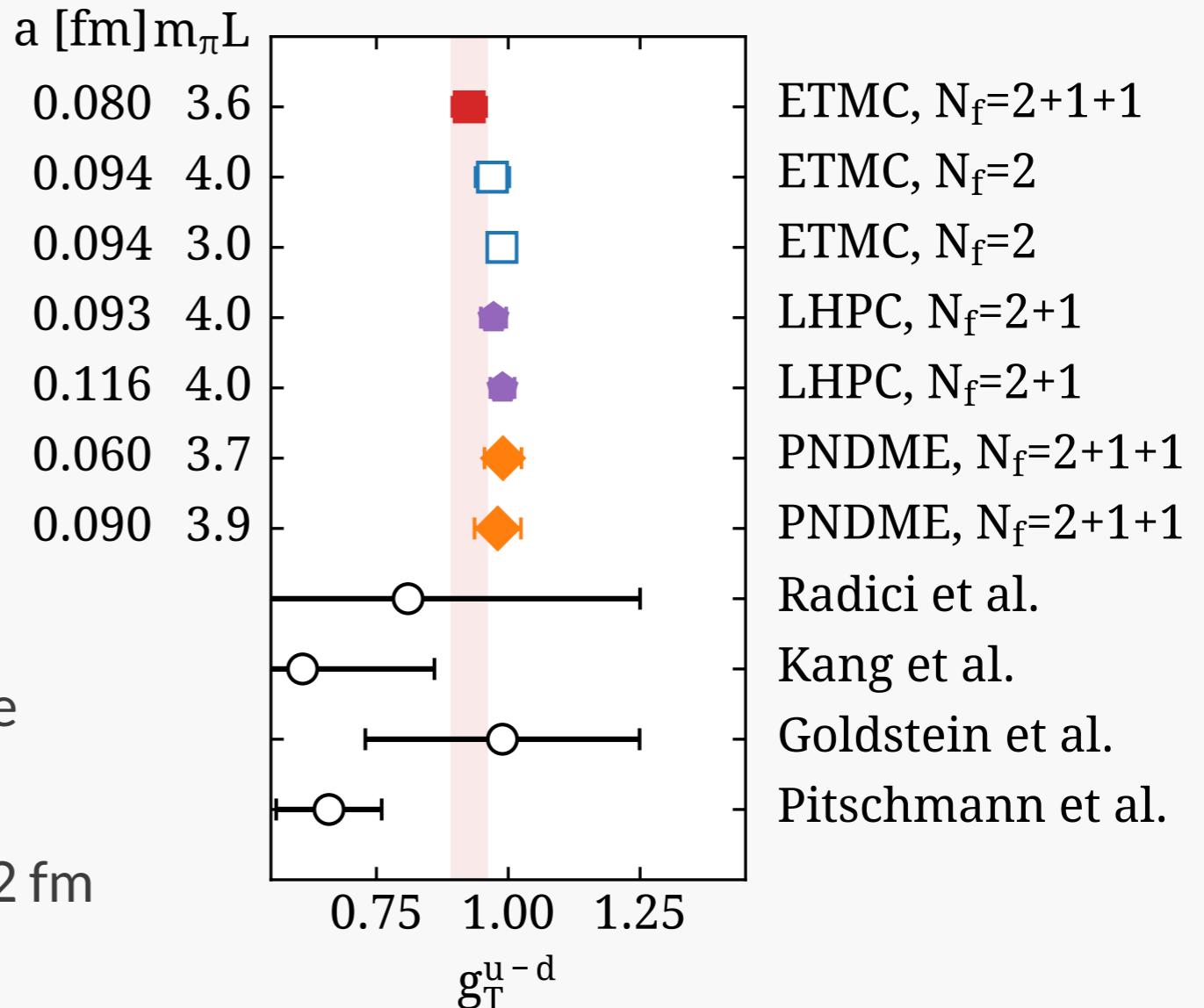


Tensor charge

Isovector tensor charge



- Precise results from multiple lattice
- Volumes between $L=4.4$ to 5.8 fm
- Lattice spacing spanning 0.06 - 0.12 fm



Moments of PDFs

Isovector matrix element of 1st-derivative operators

- Unpolarized (momentum fraction)

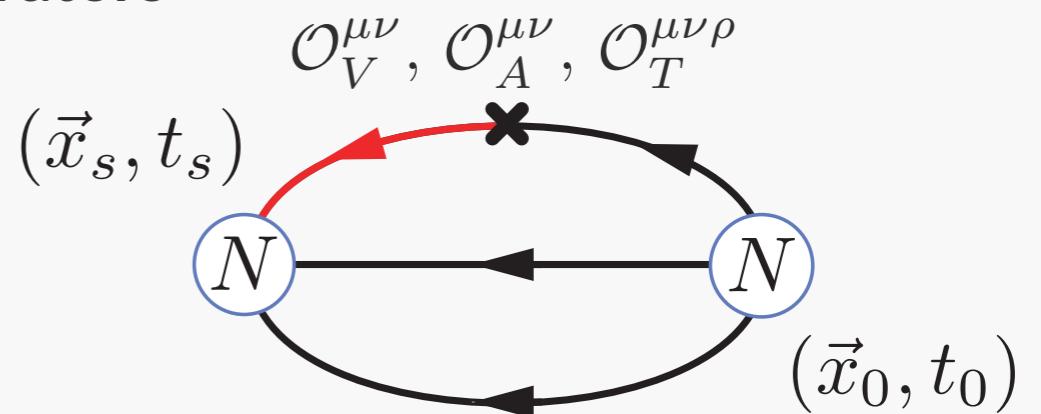
$$\mathcal{O}_V^{\mu\nu} = \bar{\psi} \gamma^{\{\mu} \overleftrightarrow{D}^{\nu\}} \psi, \Pi_V^{44}(\Gamma_0) = -\frac{3m_N}{4} \langle x \rangle_{u-d}$$

- Helicity

$$\mathcal{O}_A^{\mu\nu} = \bar{\psi} \gamma_5 \gamma^{\{\mu} \overleftrightarrow{D}^{\nu\}} \psi, \Pi_A^{j4}(\Gamma_k) = -\frac{im_N}{2} \delta_{jk} \langle x \rangle_{\Delta u - \Delta d}$$

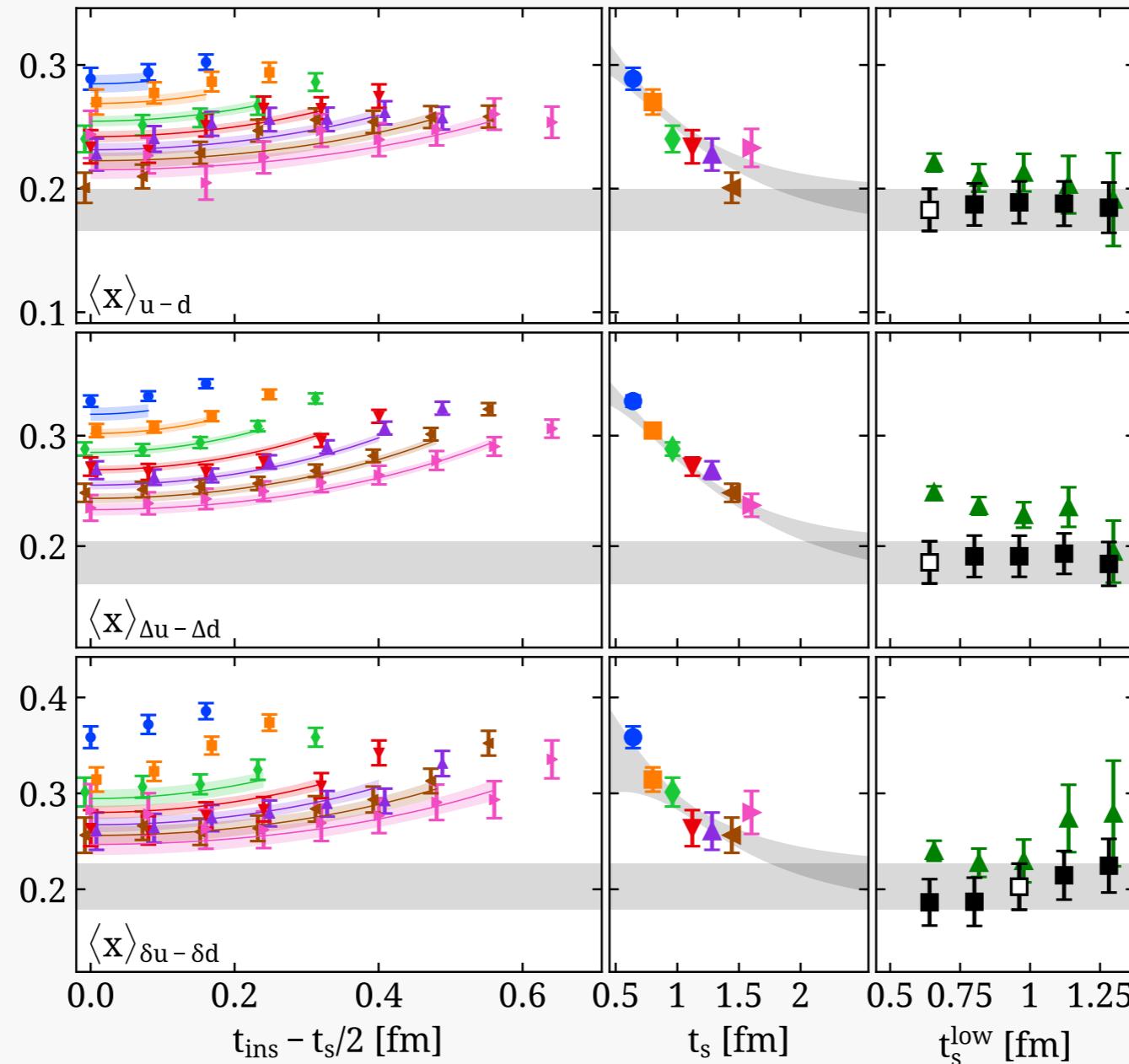
- Transversity

$$\mathcal{O}_T^{\mu\nu\rho} = \bar{\psi} \sigma^{[\mu\{\nu]} \overleftrightarrow{D}^{\rho\}} \psi, \Pi_T^{\mu\nu\rho}(\Gamma_k) = i\epsilon_{\mu\nu\rho k} \frac{m_N}{8} (2\delta_{4\rho} - \delta_{4\mu} - \delta_{4\nu}) \langle x \rangle_{\delta u - \delta d}$$



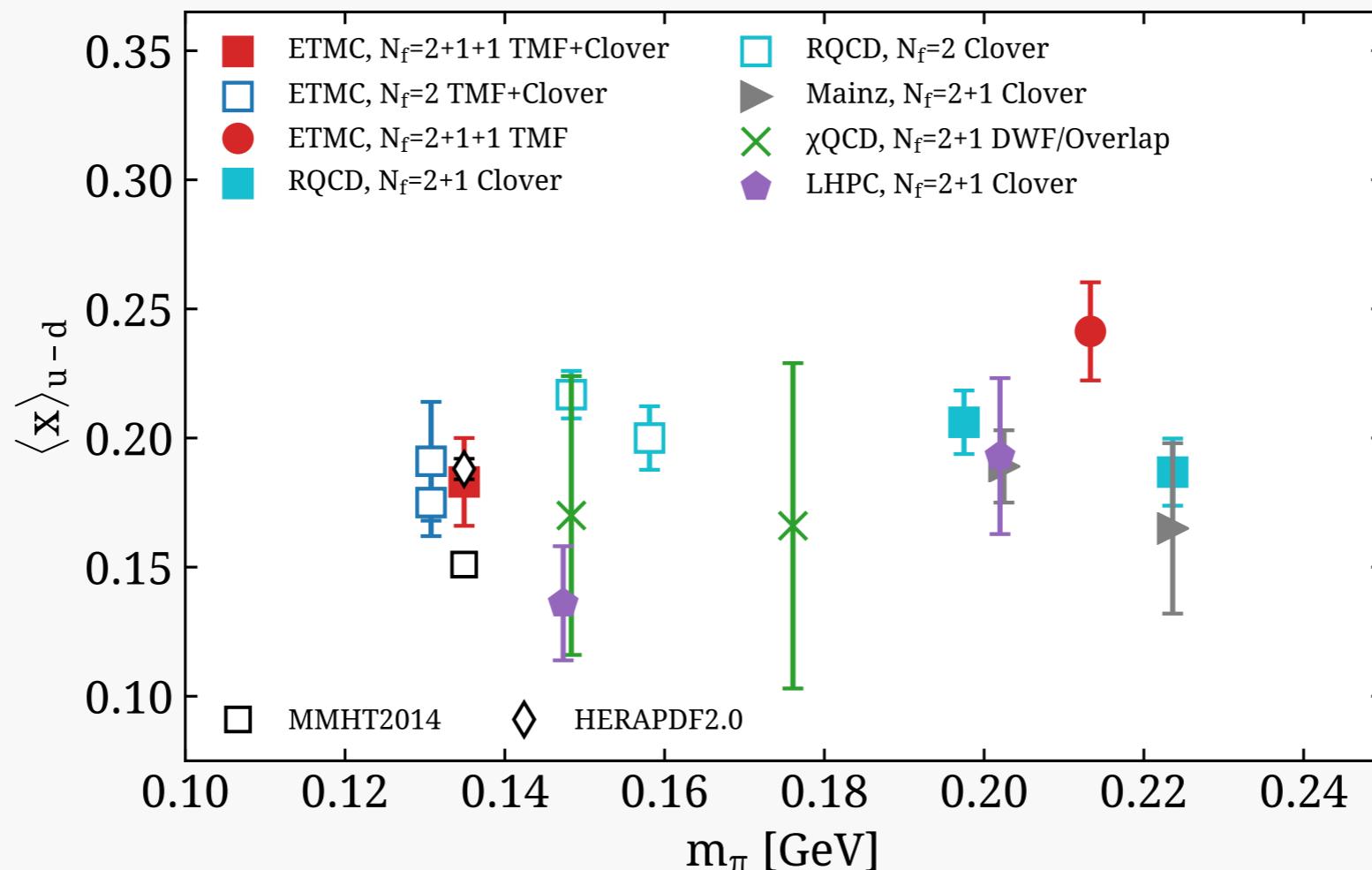
Moments of PDFs

Isovector matrix element of 1st-derivative operators



Moments of PDFs

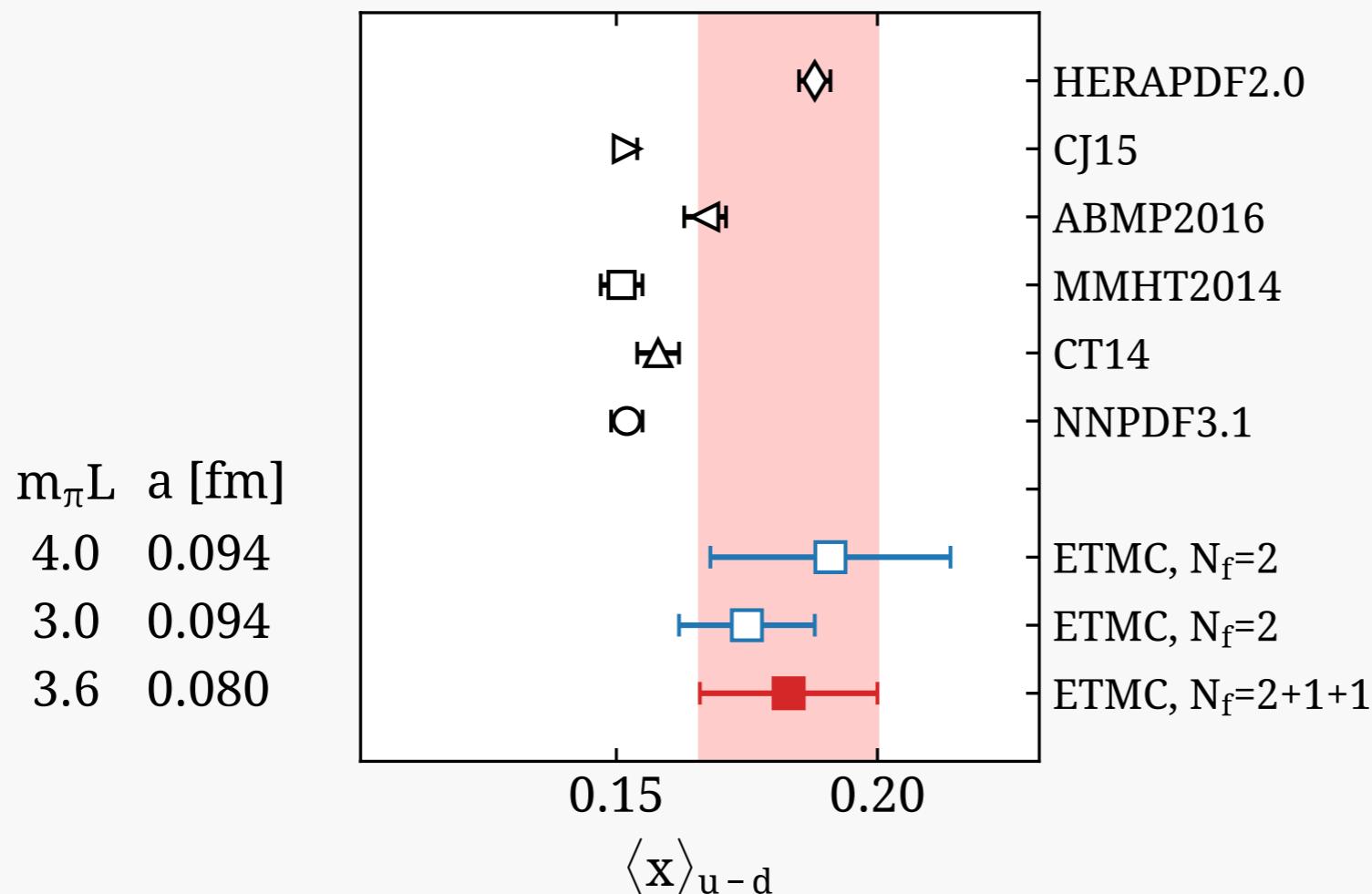
Isovector matrix element of 1st-derivative operators



- New results directly at the physical point
- Physical point results within phenomenological spread

Moments of PDFs

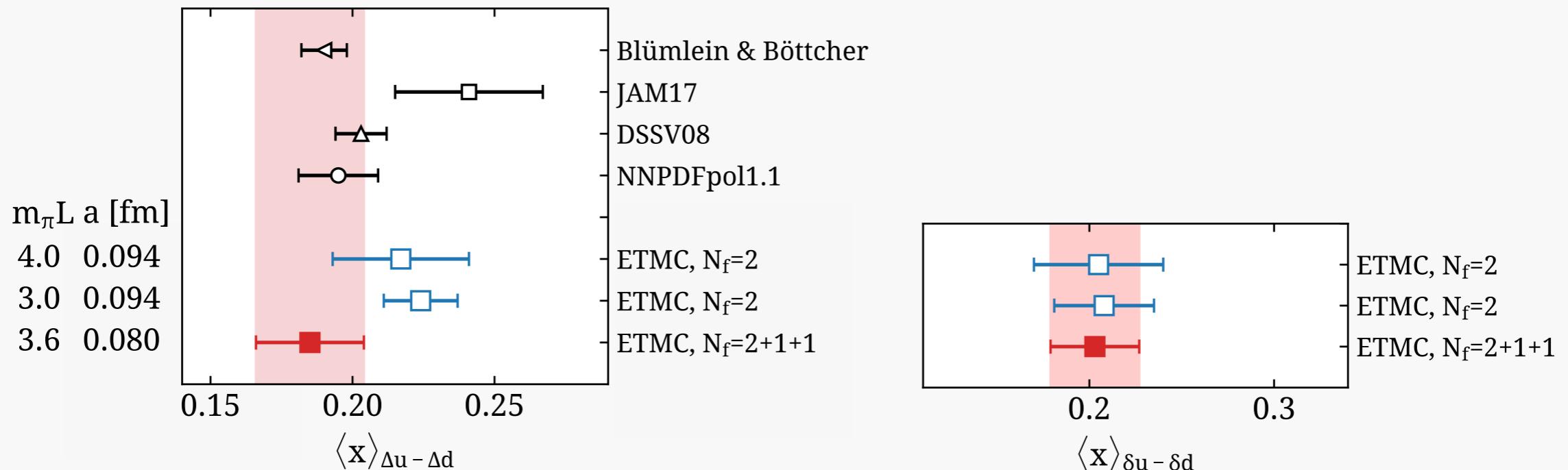
Isovector matrix element of 1st-derivative operators



- Check of volume effects
- Slightly higher value compared to most phenomenological extractions

Moments of PDFs

Isovector matrix element of 1st-derivative operators



- Not shown: One other lattice study at 150 MeV: RQCD, arXiv:1812.08256, PRD
 - Extracted from single separation ~ 1.1 fm
 - Consistent with our plateau at similar separation

Nucleon Generalized Form-Factors

Matrix element:

$$\langle N(p', s') | \mathcal{O}_{V,A}^{\mu\nu} | N(p, s) \rangle = \bar{u}_N(p', s') \frac{1}{2} [\dots] u_N(p, s)$$

Three vector and two axial GFFs:

$$\text{Vector : } A_{20}(q^2) \gamma^{\{\mu} P^{\nu\}} + B_{20}(q^2) \frac{i\sigma^{\{\mu\alpha} q_\alpha P^{\nu\}}}{2m_N} + C_{20}(q^2) \frac{1}{m_N} q^{\{\mu} q^{\nu\}}$$

$$\text{Axial : } \tilde{A}_{20}(q^2) \gamma^{\{\mu} P^{\nu\}} \gamma^5 + \tilde{B}_{20}(q^2) \frac{q^{\{\mu} P^{\nu\}}}{2m_N} \gamma^5$$

Ji spin sum:

$$J^q = \frac{1}{2} [A_{20}^q(0) + B_{20}^q(0)]$$

$A_{20}^{u-d}(0) = \langle x \rangle_{u-d}$: directly calculated at $Q^2=0$

$B_{20}^{u-d}(0)$: need to model $B_{20}^{u-d}(Q^2)$ and take $Q^2 \rightarrow 0$

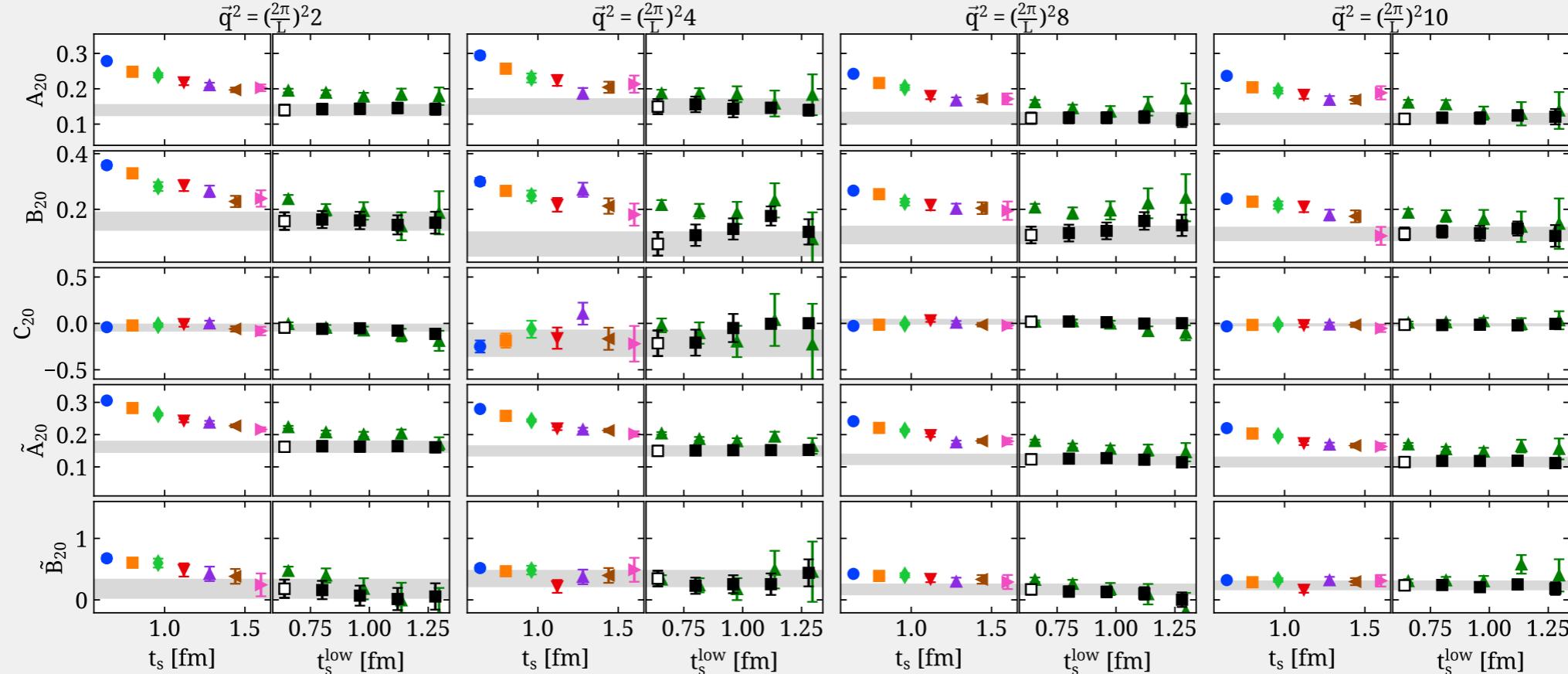
Nucleon Generalized Form-Factors

Solve via SVD of matrix of kinematics:

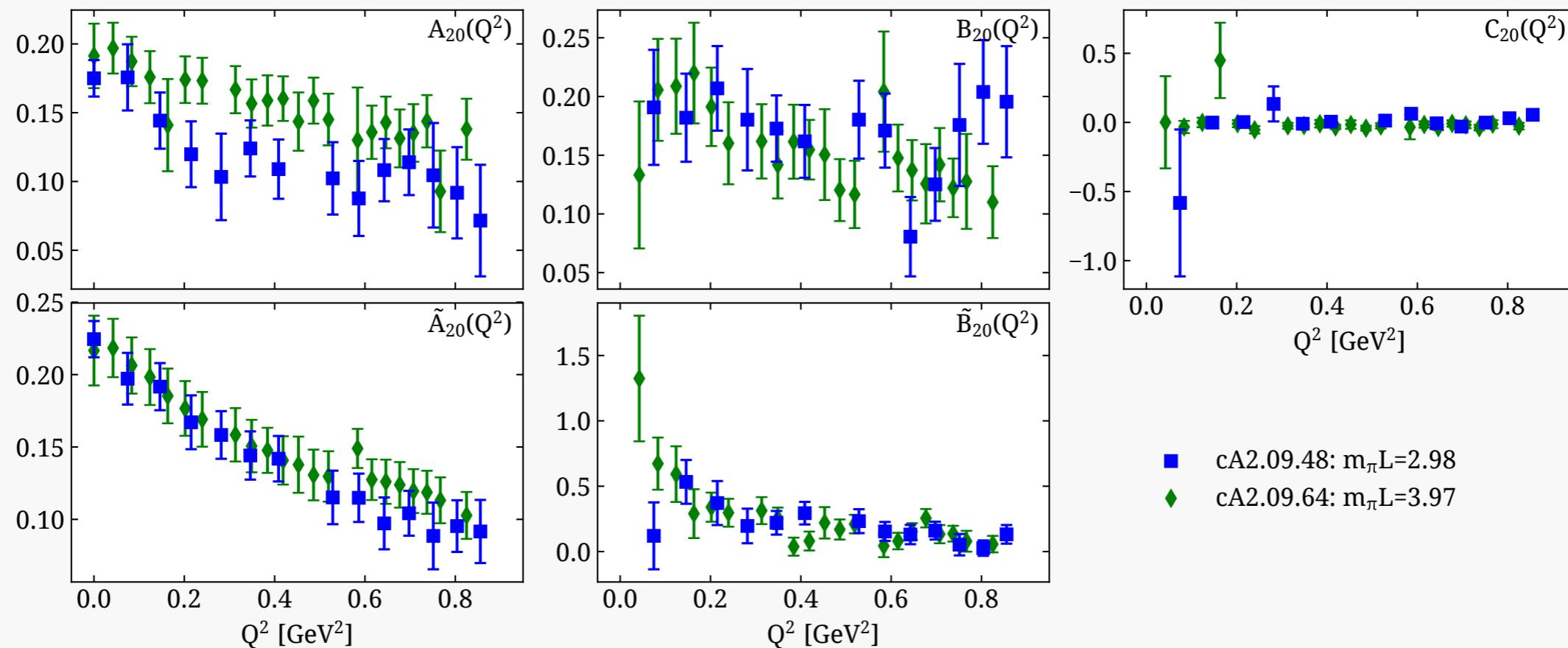
$$\Pi^{\mu\nu}(\Gamma; \vec{q}) = \mathcal{G}^{\mu\nu}(\Gamma; \vec{q}) F(Q^2)$$

Π lattice measurements, \mathcal{G} kinematics, F vector of GFFs

Excited state analysis as charges but for each Q^2 separately



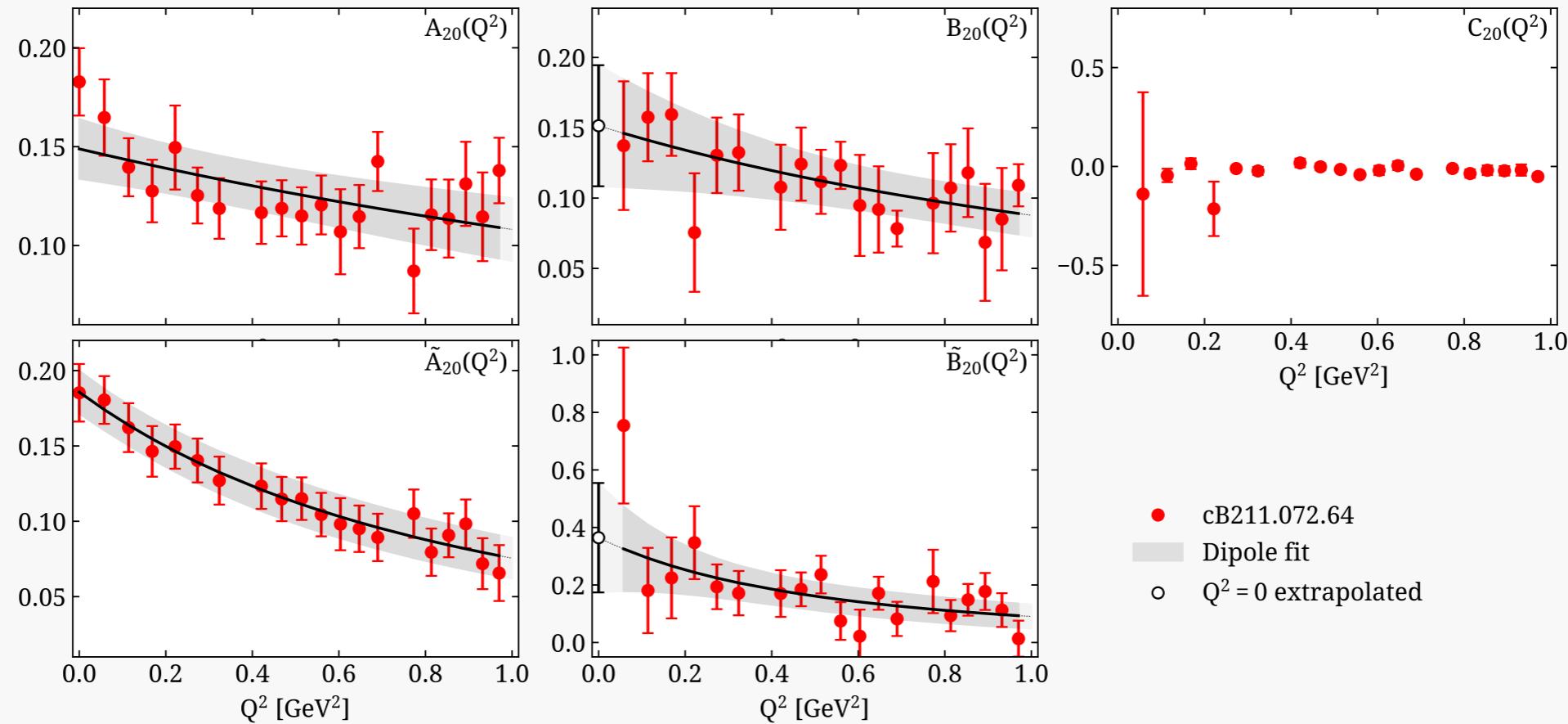
Nucleon Generalized Form-Factors



GFFs finite volume effect study using $N_f=2$ twisted mass

- No detectable effects from the init volume between $m_\pi L \approx 3$ and 4

Nucleon Generalized Form-Factors



$N_f=2+1+1$ at physical pion mass

- Dipole fits model well B_{20} and \tilde{A}_{20}
- Tripole fits also model well B_{20} and \tilde{B}_{20}

$$J^{u-d} = \frac{1}{2}[A_{20}^{u-d}(0) + B_{20}^{u-d}(0)] = 0.167(24)(04)$$

Summary

- Nucleon moments of PDFs
 - Local matrix elements of nucleon
 - Physical pion masses available by multiple collaborations
 - Disconnected contributions for individual u , d , s , c contributions
 - Analyses focusing on ensuring ground-state dominance
- Gluonic contributions also available (not covered here)
- Results available at physical quark masses:
 - Nucleon charges and moments of PDFs comparable to experiment
 - Flavor separation thanks to techniques for disconnected contributions
 - Momentum-dependence of moments (FFs and GFFs)
- Ongoing:
 - Finer lattices and larger volumes

Contributors

ETM Collaboration



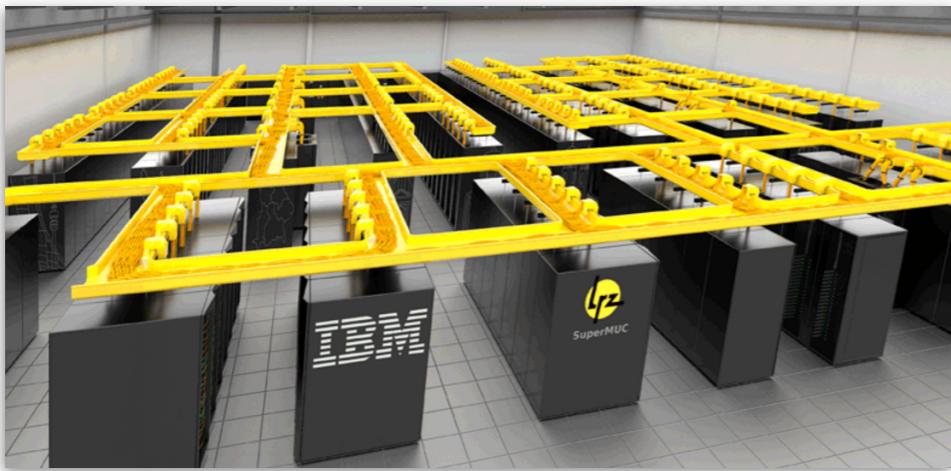
Nucleon Structure

C. Alexandrou, [S. Bacchio](#), M. Constantinou,
J. Finkenrath, K. Hadjyiannakou, K. Jansen,
[C. Lauer](#), [A. Scapellato](#), F. Steffens, A. Vaquero

[Cyprus](#) (Univ. of Cyprus, Cyprus Inst.), [France](#) (Orsay, Grenoble), [Germany](#) (Berlin/Zeuthen, Bonn, Frankfurt, Hamburg, Jena, Münster), [Italy](#) (Rome I, II, III), [Netherlands](#) (Groningen), [Poland](#) (Poznan), [Switzerland](#) (Bern), [UK](#) (Liverpool), [US](#) (Temple, PA)

Acknowledgements

Gauge Field generation:
SuperMUC @ LRZ



Propagators & Contractions:
Piz Daint @ CSCS



- tmLQCD: github.com/etmc/tmLQCD
- DDalphaAMG adapted to twisted mass: github.com/sbacchio/DDalphaAMG

- QUDA Multi-Grid
- Custom contraction code: github.com/ETMC-QUADA/quda-QKXTM-Multigrid-PlugIn

NextQCD, EXCELLENCE/1918/0129

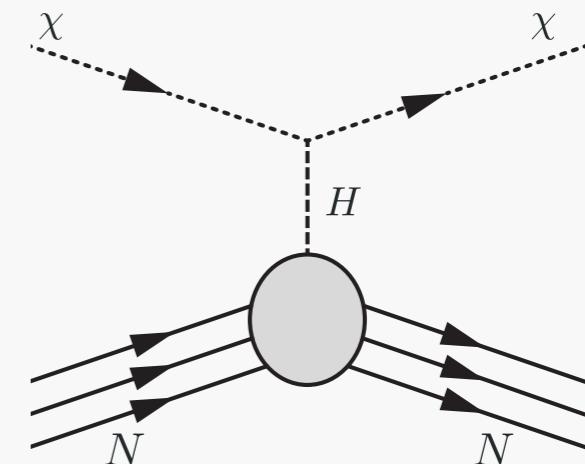


Ευρωπαϊκή Ένωση
Ευρωπαϊκά Διαρθρωτικά
και Επενδυτικά Ταμεία

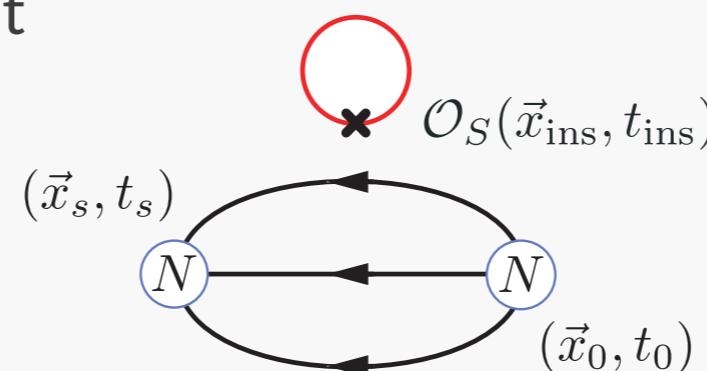
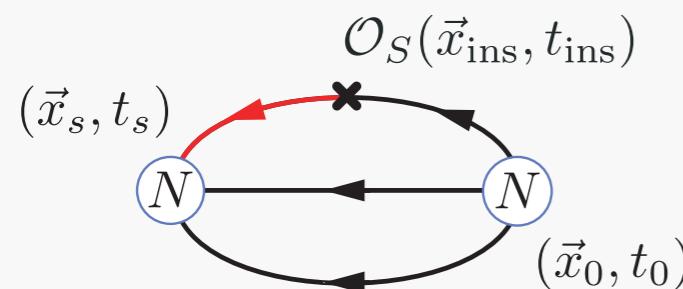
Backup

Nucleon σ -terms

- Pion nucleon σ -term: $\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle$
- Strange σ -term: $\sigma_s = m_s \langle N | \bar{s}s | N \rangle$
- Scattering cross sections of scalars with nucleon
(e.g. neutralino through Higgs)



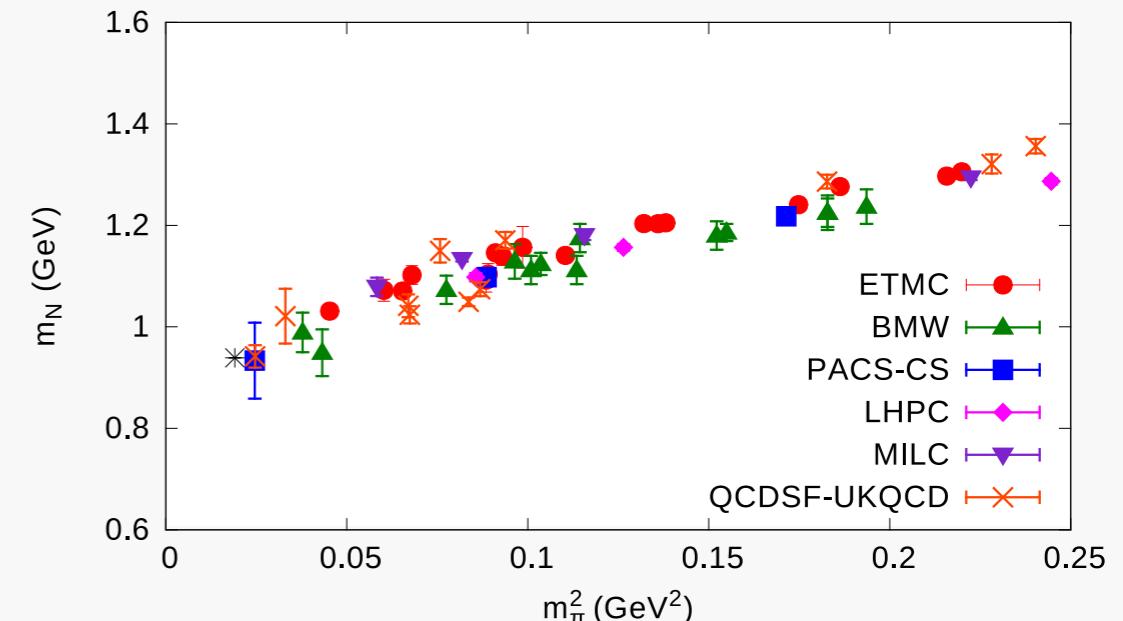
Direct: through matrix element



Feynman - Hellmann: dependence on quark mass

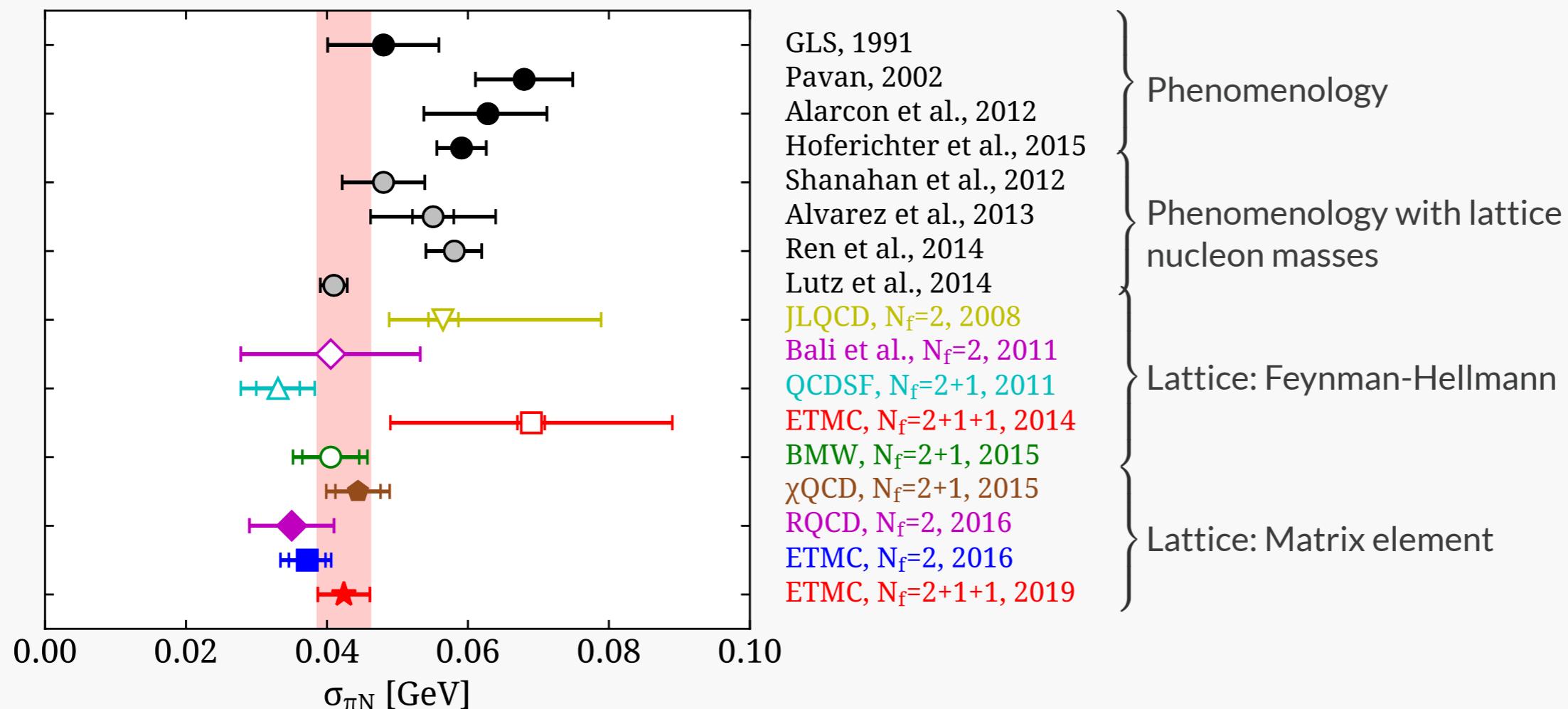
- Requires modelling of m_q dependence
- Weak m_s dependence

Poster by W. Soeldner, spectrum and σ -terms from QCDSF



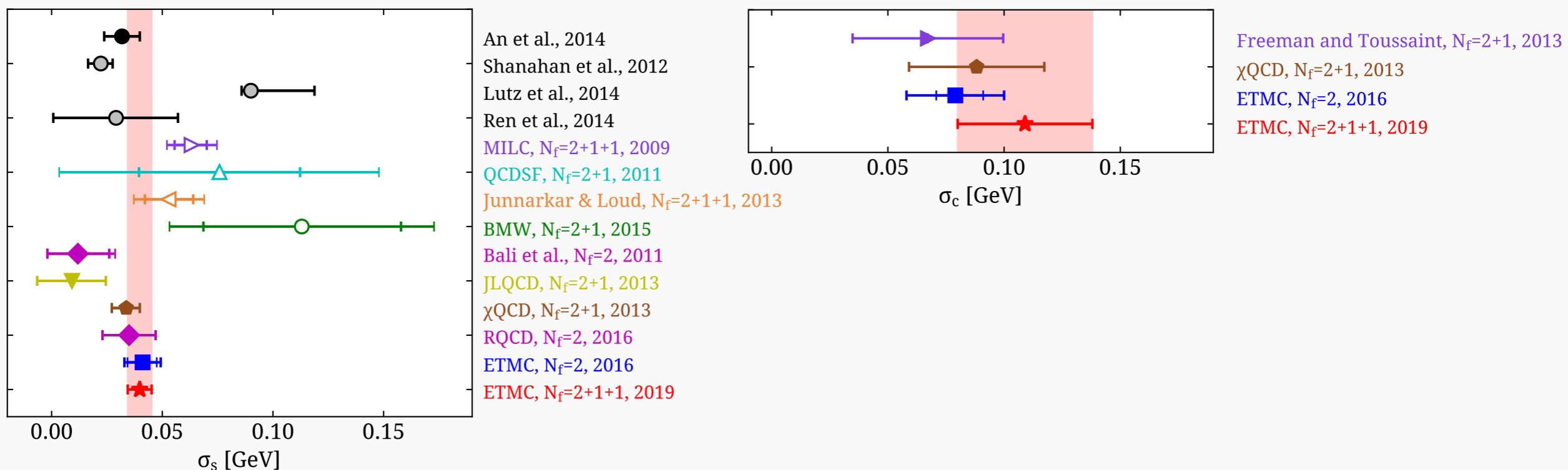
Nucleon σ -terms

Light σ -term $\sigma_{\pi N}$



Nucleon σ -terms

Good signal also for strange and charm σ -terms



- General consistency between lattice results and experimental determinations

Nucleon Electromagnetic Form-Factors

Matrix element:

$$\langle N(p', s') | j^\mu | N(p, s) \rangle = \sqrt{\frac{M_N^2}{E_N(\mathbf{p}') E_N(\mathbf{p})}} \bar{u}(p', s') \mathcal{O}^\mu u(p, s)$$

$$\mathcal{O}^\mu = \gamma_\mu F_1(q^2) + \frac{i\sigma_{\mu\nu}q^\nu}{2M_N} F_2(q^2), \quad q = p' - p$$

Sachs form-factors:

$$G_M(q^2) = F_1(q^2) + F_2(q^2)$$

$$G_E(q^2) = F_1(q^2) + \frac{q^2}{(2M_N)^2} F_2(q^2)$$

Isovector & Isoscalar combinations:

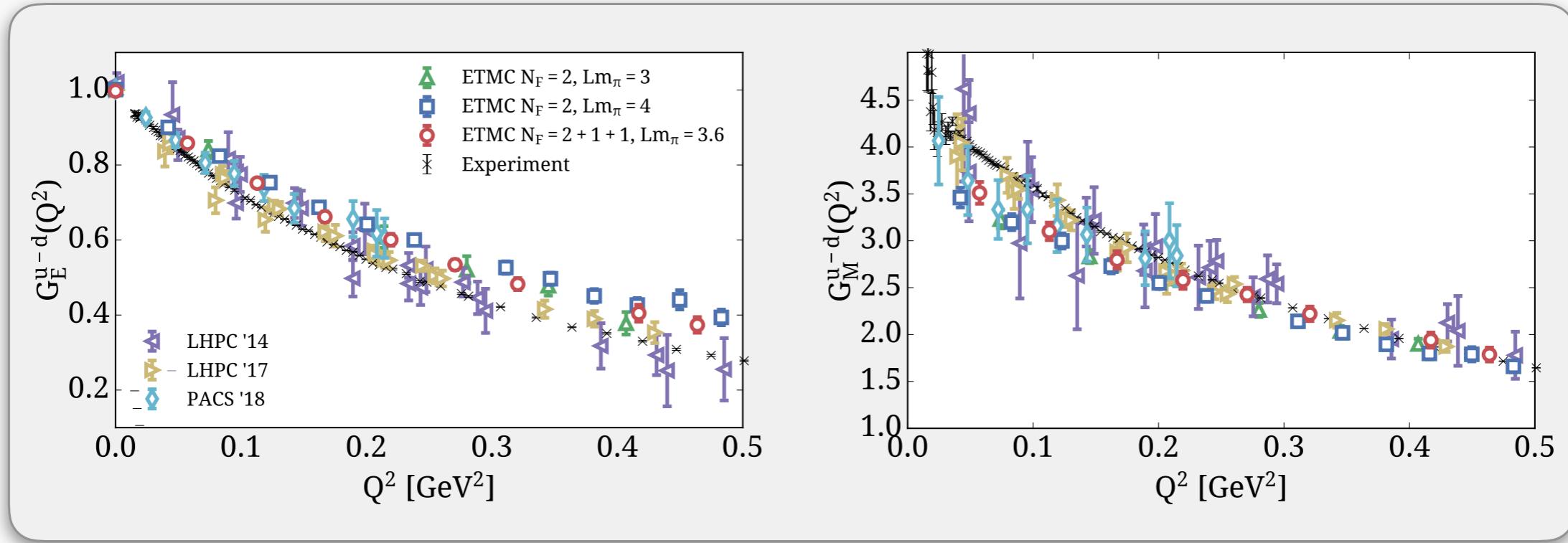
$$j_\mu^v = \bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d, \quad j_\mu^s = \bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d$$

$$F^p - F^n = F^u - F^d$$

Assuming flavour isospin symmetry

$$F^p + F^n = \frac{1}{3}(F^u + F^d)$$

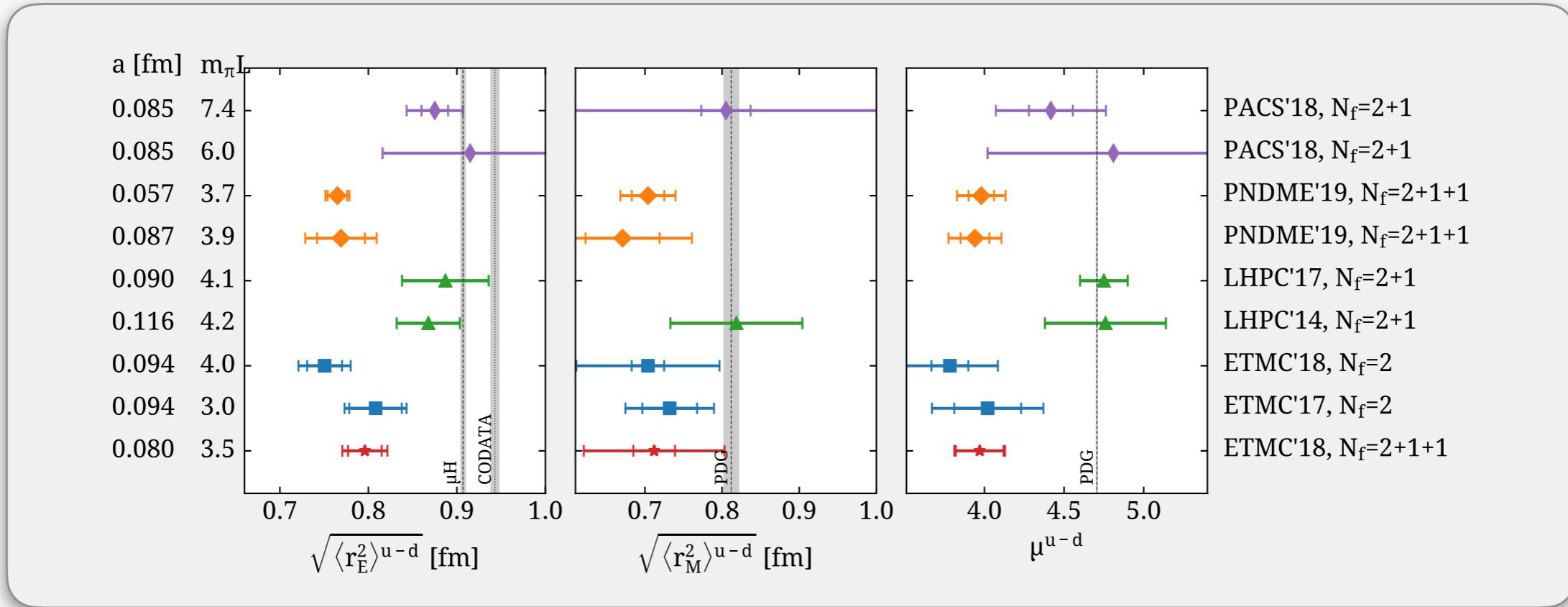
Nucleon Electromagnetic Form-Factors



Isovector EM form-factors

- Multiple groups with physical pion mass
- G_E : slight tension at high Q^2
- G_M : slight tension at small Q^2

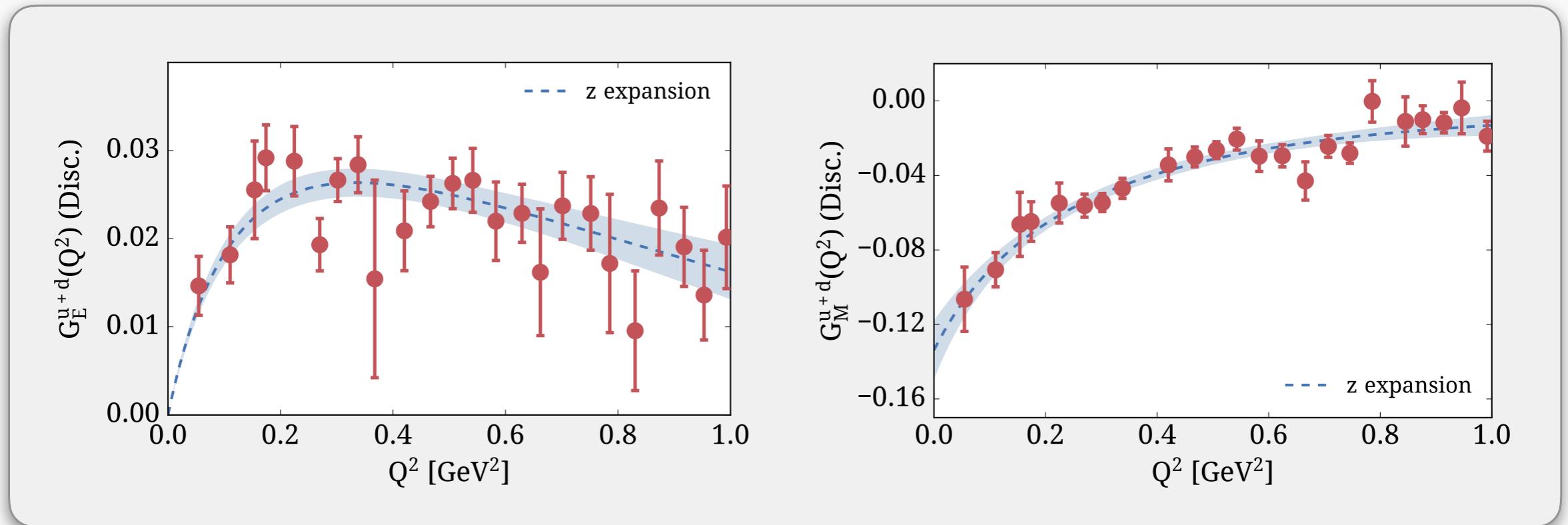
Nucleon Electromagnetic Form-Factors



Isovector EM form-factors

- Estimation of all systematics still ongoing
- Continuum and volume extrapolations still needed

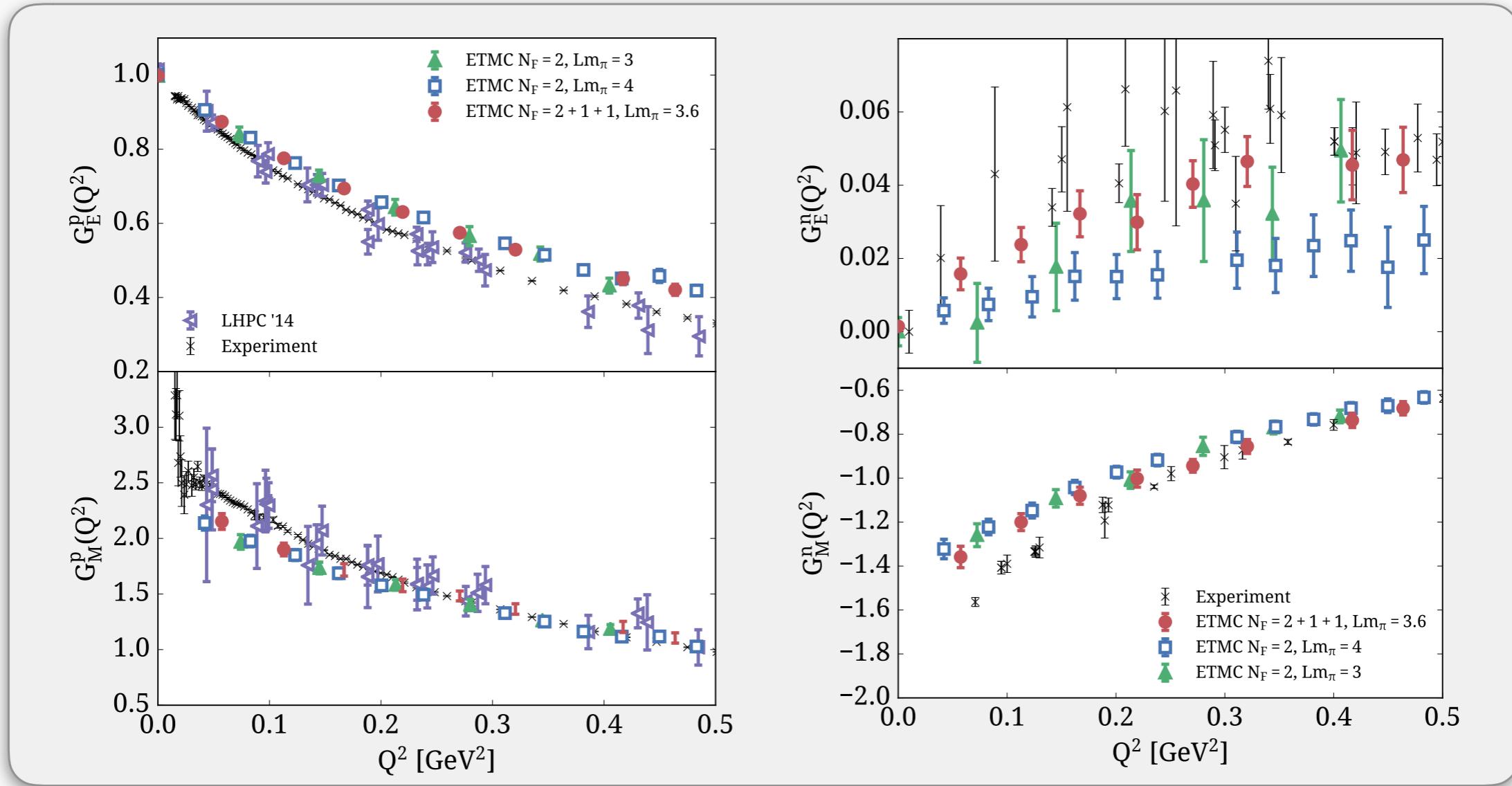
Nucleon Electromagnetic Form-Factors



Proton/neutron separated: need disconnected diagrams

- Good signal thanks to hierarchical probing and use of boosted frames
- Small in magnitude (few percent level)

Nucleon Electromagnetic Form-Factors



Proton/neutron separated EM form-factors

- Including disconnected; non-negligible effect for neutron G_E
- G_E : slight tension at high Q^2
- G_M : slight tension at small Q^2

Axial Form Factors

★ Axial and induced pseudo-scalar

$$\langle N(p', s') | A_\mu^3 | N(p, s) \rangle = i \sqrt{\frac{m_N^2}{E_N(\vec{p}') E_N(\vec{p})}} \bar{u}(p', s') [\gamma_\mu \gamma_5 G_A(q^2) + \frac{q_\mu \gamma_5}{2m_N} G_p(q^2)] \frac{1}{2} u_N(p, s)$$

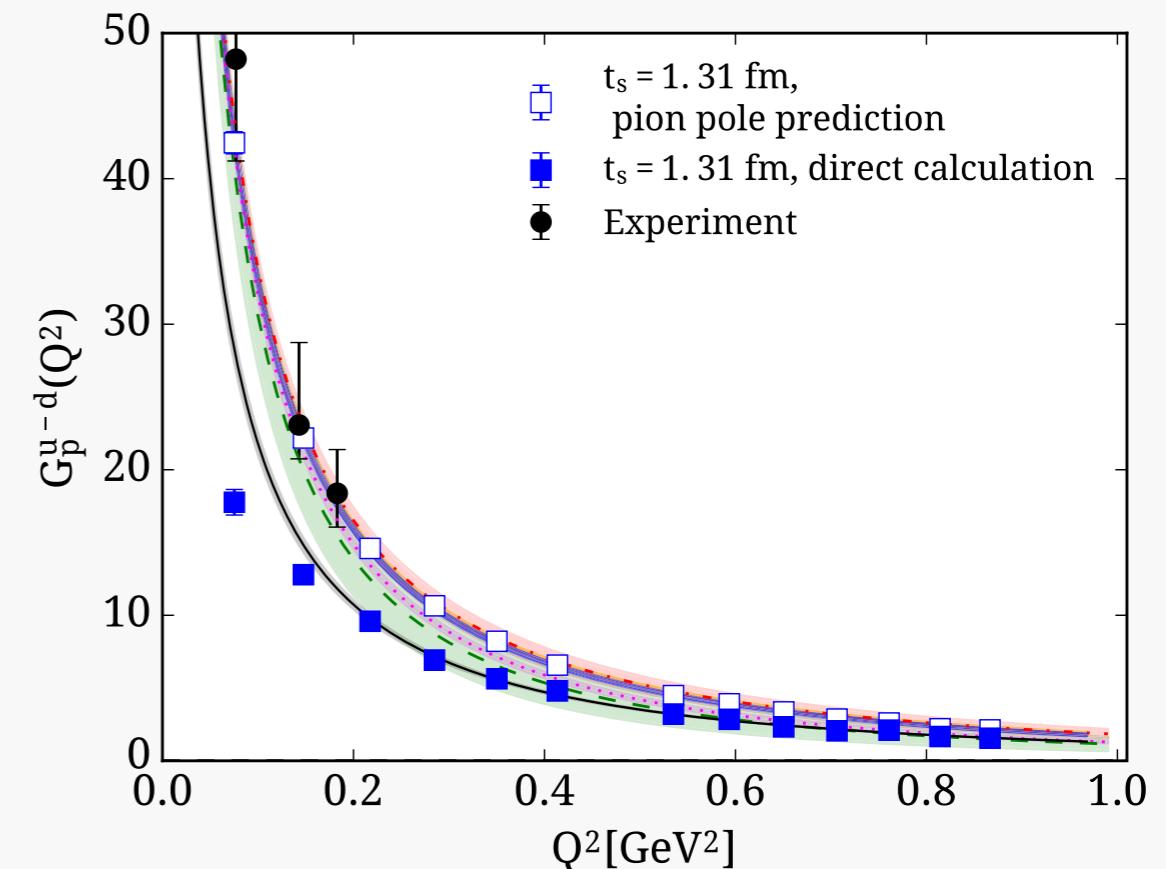
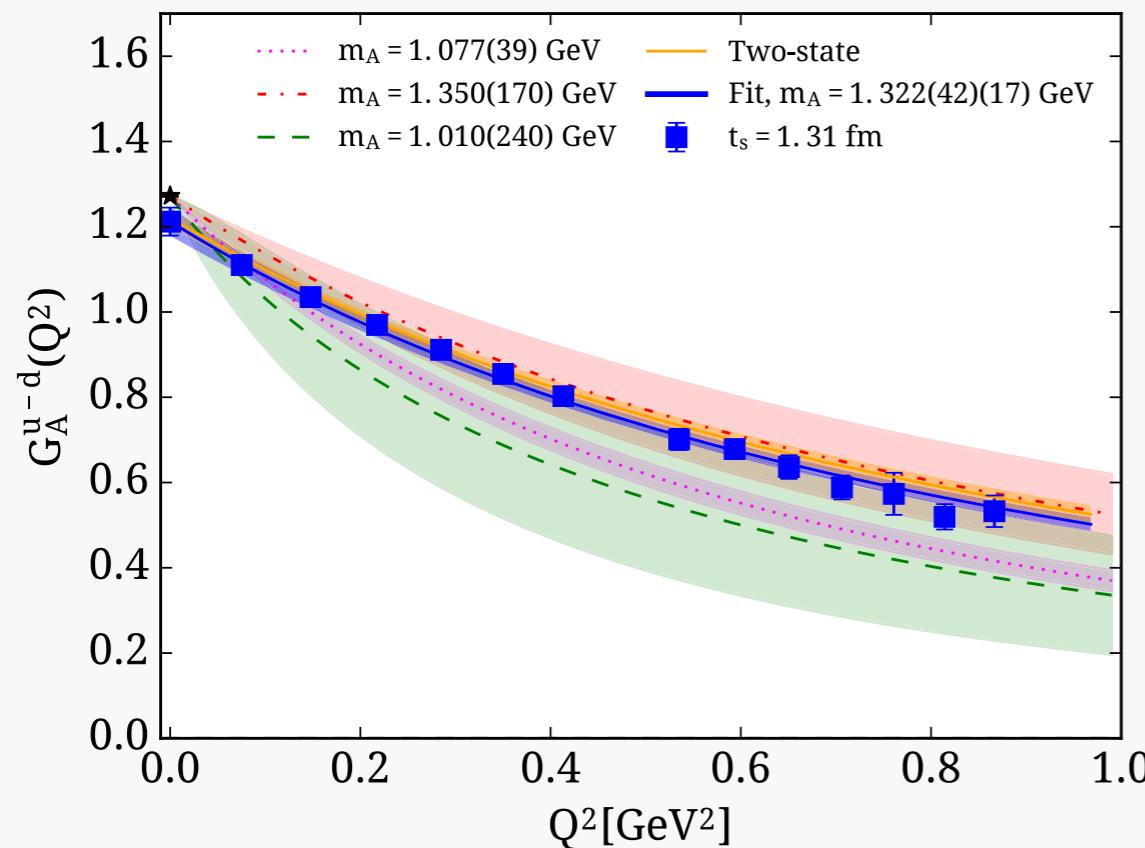
with:

$$A_\mu^3(x) = \bar{\psi}(x) \gamma_\mu \gamma_5 \frac{\tau^3}{2} \psi(x), \text{ and } \psi = \begin{pmatrix} u \\ d \end{pmatrix}$$

- Known to less accuracy experimentally (e.g. compared to electromagnetic)
 - Via elastic scattering: $\nu_\mu + n \rightarrow \mu^- + p$
 - Via charged pion electroproduction
- Required in neutrino oscillation experiments. Traditionally modelled with a dipole form:
$$G_A(Q^2) = \frac{g_A}{(1 + \frac{Q^2}{M_A^2})^2}$$
to extract the “axial radius”: $\langle r_A^2 \rangle = \frac{12}{M_A^2}$

- From ν -scattering: $M_A = 1.026(21)$ GeV
- MiniBooNE (2002): $M_A = 1.35(17)$ GeV

Axial Form Factors

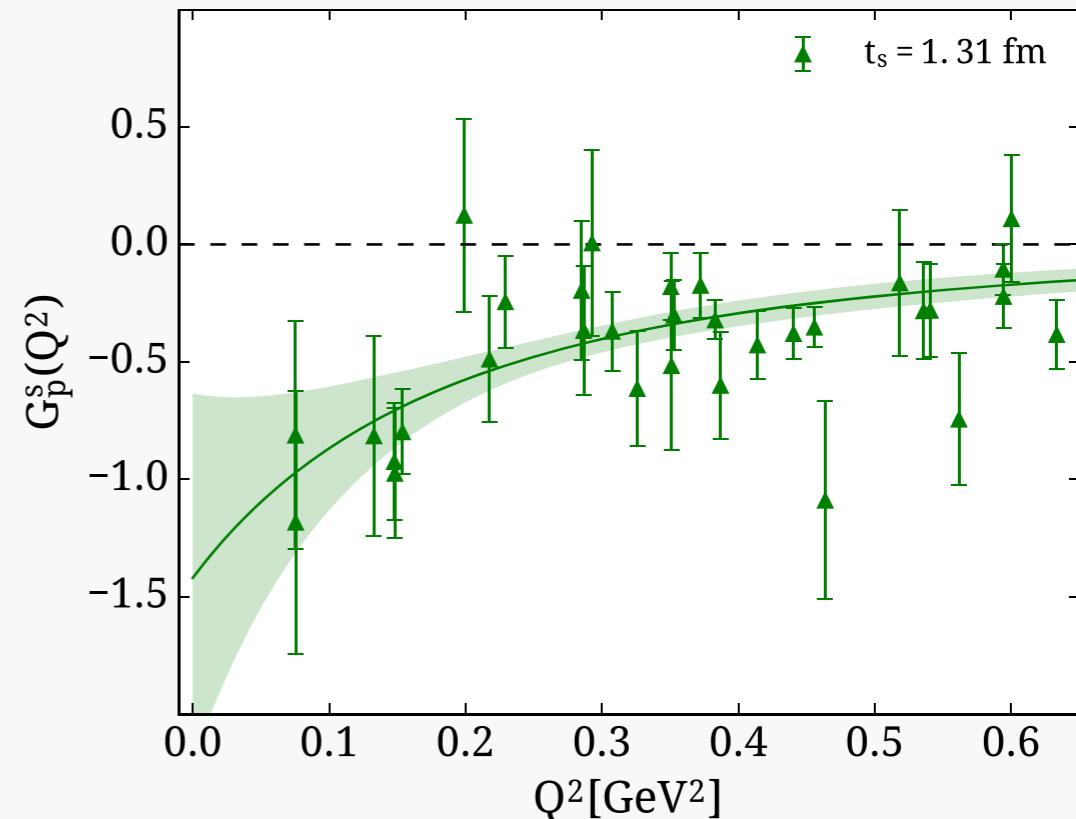
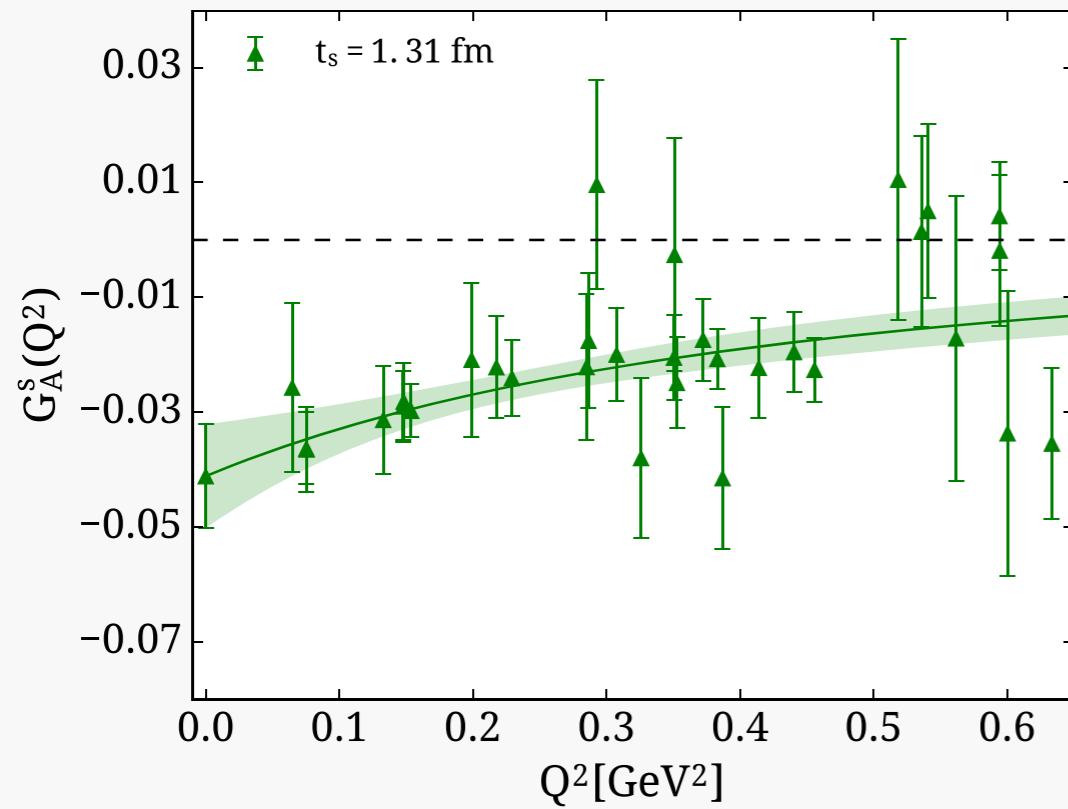


- Axial and induced pseudo scalar from one ensemble with $m_\pi = 130$ MeV
- Axial form-factor within bands of experimental determinations
- Induced pseudo scalar does not follow the pion pole prediction

$$G_p(Q^2) = G_A(Q^2) \frac{C}{Q^2 + m_\pi^2}$$

arXiv:1705.03399, PRD

Axial Form Factors

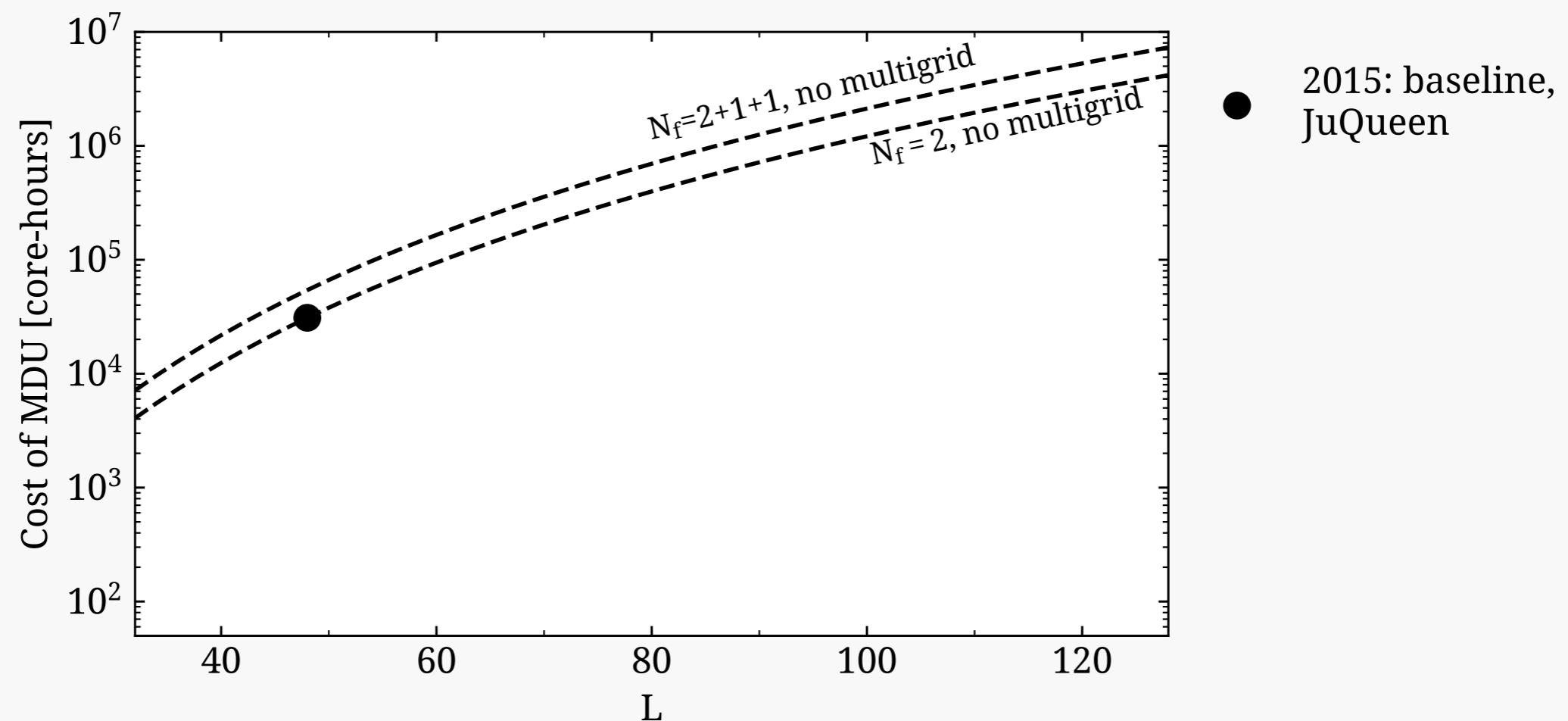


- Strange components from disconnected contributions
- Negative and non-zero signal

Lattice QCD — Large-scale simulations

A combination of

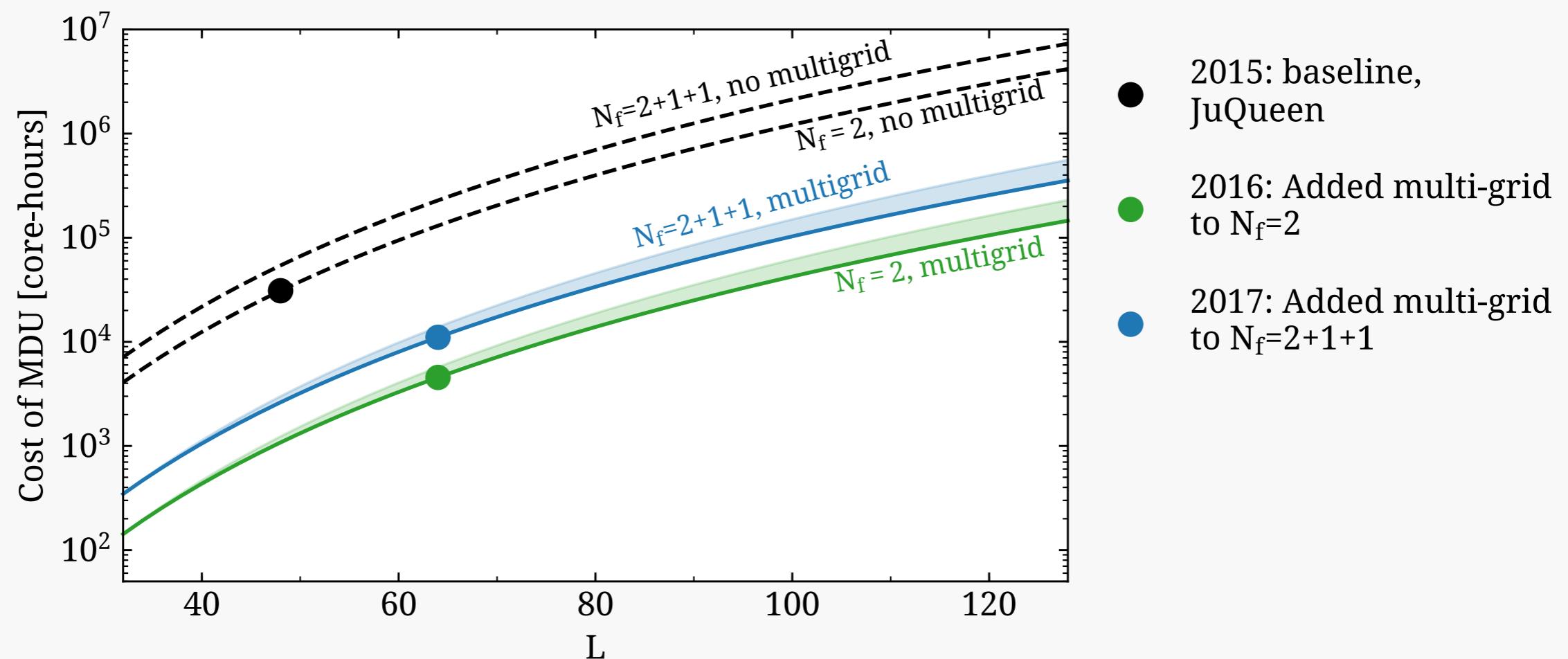
- Use of advanced computers
- Development of new algorithms



Lattice QCD — Large-scale simulations

A combination of

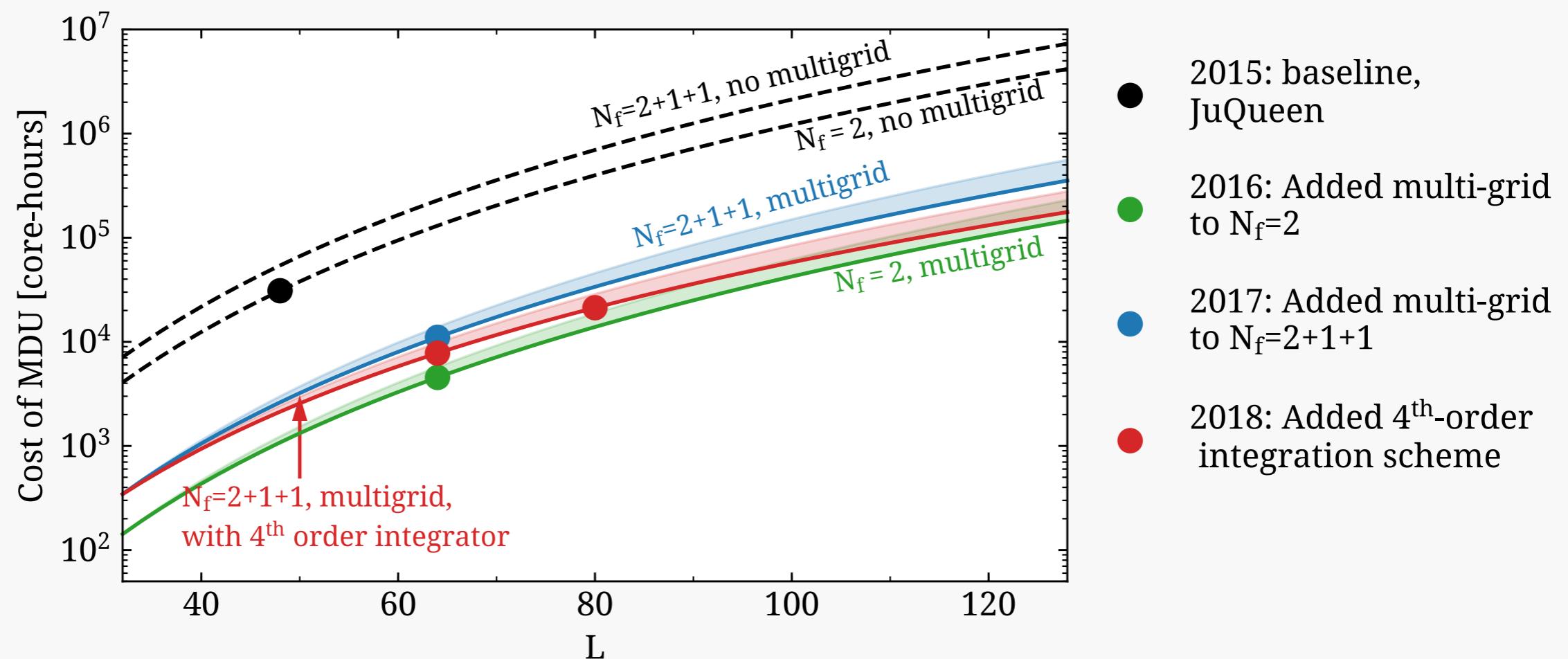
- Use of advanced computers
- Development of new algorithms



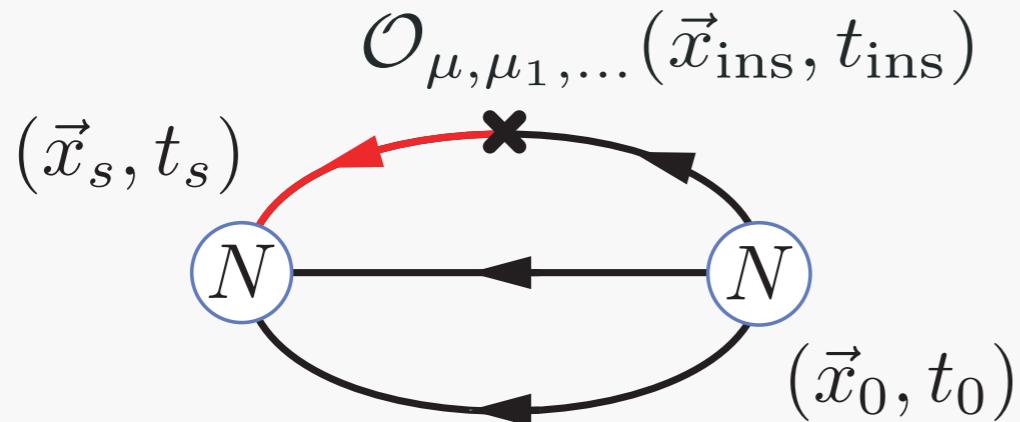
Lattice QCD — Large-scale simulations

A combination of

- Use of advanced computers
- Development of new algorithms



Setup



Connected:

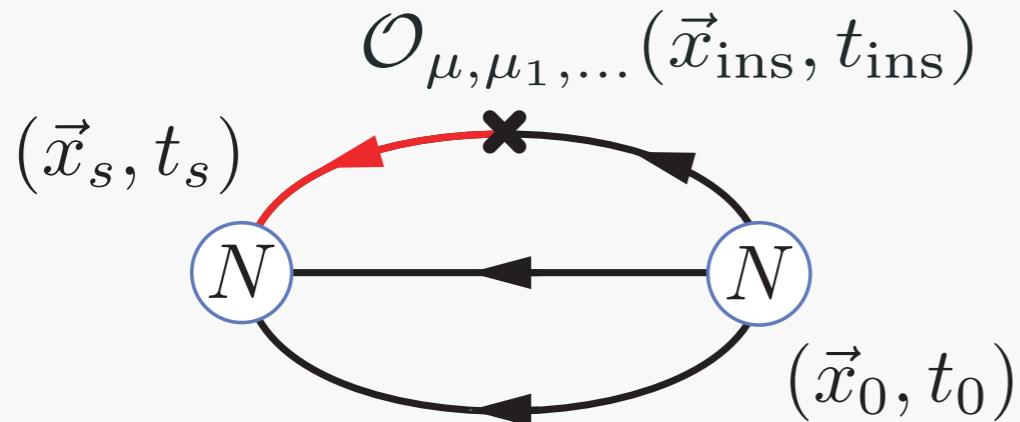
- Sequential inversion through the sink
- Fix: Sink-source separation (t_s), nucleon polarisation (Γ), sink momentum p'

t_s/a	$N_{\text{src}} \times N_{\text{conf}}$		
	cB211.072.64	cA2.09.48	cA2.09.64
8	1×750	—	—
10	2×750	16×578	—
12	4×750	16×578	16×333
14	6×750	16×578	16×515
16	16×750	88×530*	32×515
18	48×750	88×725*	—
20	64×750	—	—
2-point	264×750	100×2153	32×515

- Four polarisations Γ_0, Γ_k
- Sink momentum fixed to $\vec{p}' = \vec{0}$
- More statistics for two-point function from disconnected calculation

* Only for Γ_0

Setup



Connected:

- Sequential inversion through the sink
- Fix: Sink-source separation (t_s), nucleon polarisation (Γ), sink momentum p'

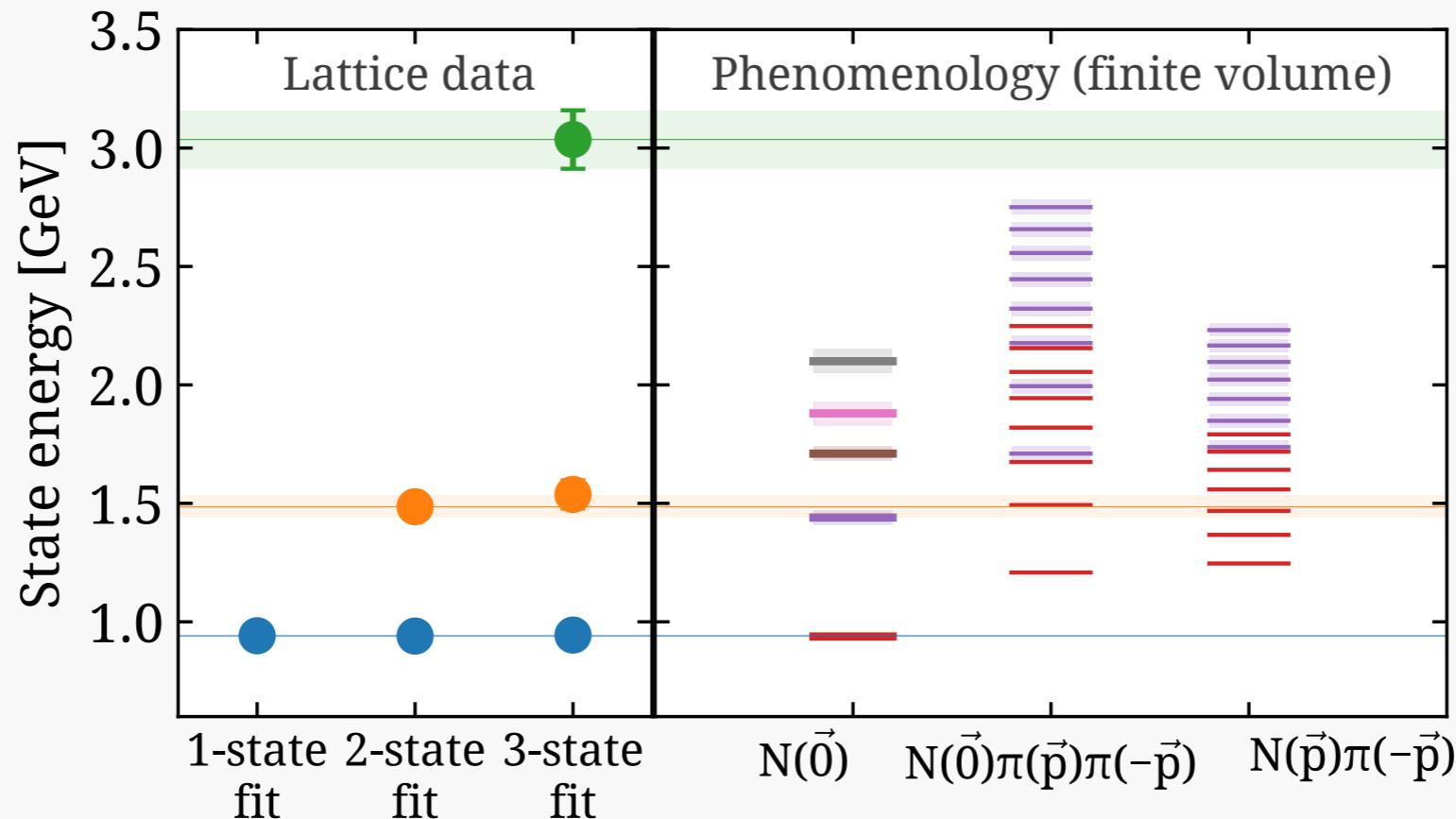
t_s/a	$N_{\text{src}} \times N_{\text{conf}}$		
	cB211.072.64	cA2.09.48	cA2.09.64
8	1×750	—	—
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16	<u>16×750</u> ×4	88×530*	32×515
18	48×750	88×725*	—
20	<u>64×750</u> ×4	—	—
2-point	264×750	100×2153	32×515

- Four polarisations Γ_0, Γ_k
- Sink momentum fixed to $\vec{p}' = \vec{0}$
- More statistics for two-point function from disconnected calculation
- Increased statistics with increasing t_s

* Only for Γ_0

Treatment of excited states

- Analysis of nucleon two-point correlation function



Excited state consistent between 2- and 3-state fit