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# Nucleon Structure From Lattice QCD Simulations at the Physical Point

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# Nucleon Structure with Physical Point Ensembles

## Outline

- Matrix elements on the lattice
- Lattice methods
- $N_f=2+1+1$  ensembles at physical point (twisted mass + clover)
- Statistics and uncertainties
- Selected results

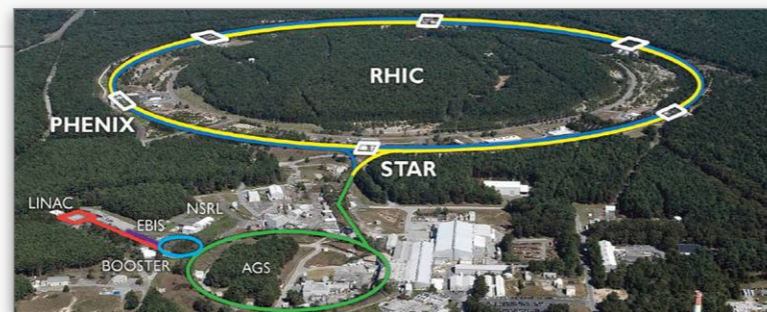
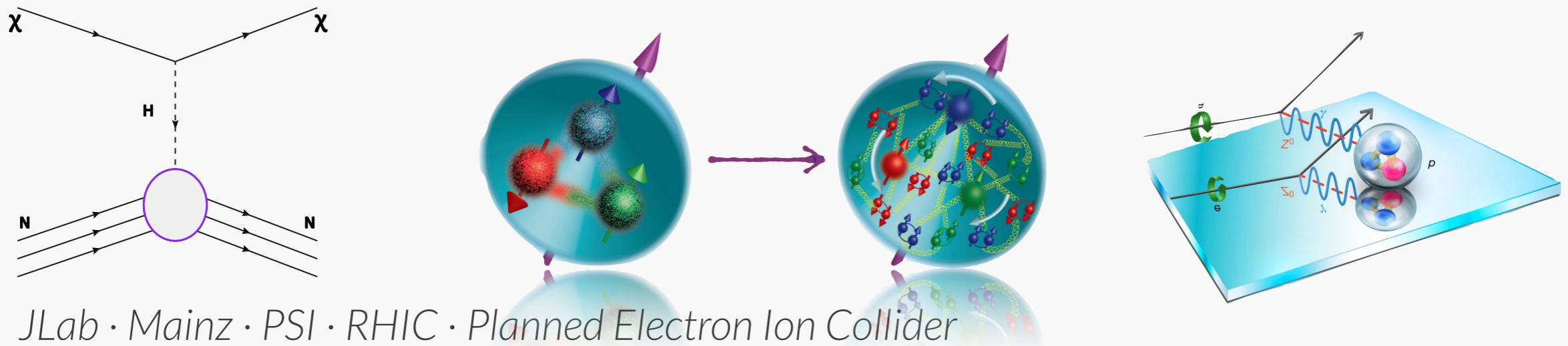


## *ETM Collaboration*

*Cyprus* (Univ. of Cyprus, Cyprus Inst.), *Germany* (Berlin/Zeuthen, Bonn, Wuppertal), *Italy* (Rome I, II, III, Parma), *Poland* (Poznan), *Switzerland* (Bern), *US* (Temple, PA)

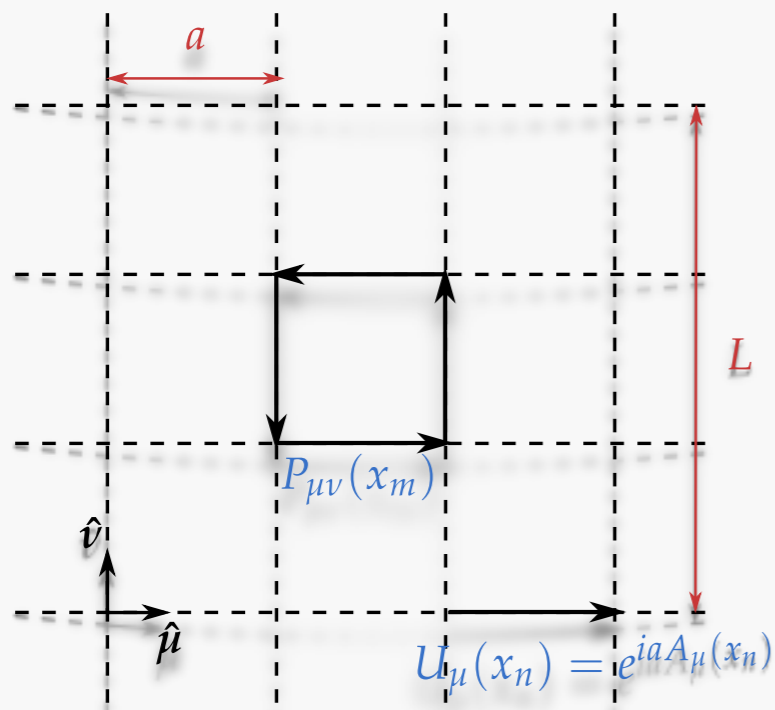
# Nucleon Matrix Elements

- Scalar and tensor charges → novel interactions/dark matter searches
- Axial matrix elements → origin of nucleon spin
- $\sigma$ -terms → mass decomposition of nucleon
- Electromagnetic form factors → radii and moments well known experimentally
- Axial form factors → PCAC and pion pole dominance relations
- Strange form factors → connect to weak charges and constraints on new physics
- Momentum fraction, moments of PDFs and GPDs, ...



# Lattice QCD — ab initio simulation of QCD

- Freedom in choice of:
  - Bare quark masses (cost increases as  $m_{PS} \rightarrow m_{\pi}$ )
  - Lattice spacing (cost increases as  $a \rightarrow 0$ )
  - Volume (cost increases as  $L^3 \rightarrow \infty$ )
- Choice of discretisation scheme; e.g. Clover, Twisted Mass, Staggered, Overlap, Domain Wall
  - Each with their own trade-offs and advantages



Eventually, **all** schemes must agree:

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

# Lattice QCD

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\mathbf{U}] \mathcal{O}(\mathbf{D}_f^{-1}[\mathbf{U}], \mathbf{u}) \left( \prod_{f=u,d,s,c} \text{Det}(\mathbf{D}_f[\mathbf{U}]) \right) e^{-S_{\text{QCD}}[\mathbf{U}]}$$

1



2



3



## Simulation

- Markov chain Monte Carlo to generate ensembles of gluon-field configurations  $\{\mathbf{U}\}$

$$P[\mathbf{U}] = \frac{1}{Z} \left( \prod_{f=u,d,s,c} \text{Det}(\mathbf{D}_f[\mathbf{U}]) \right) e^{-S_{\text{QCD}}[\mathbf{U}]}$$

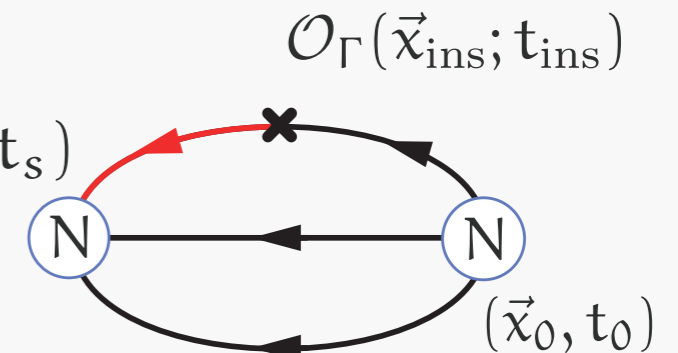
## Analysis

- Construction of hadron correlation functions on background field configurations:

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

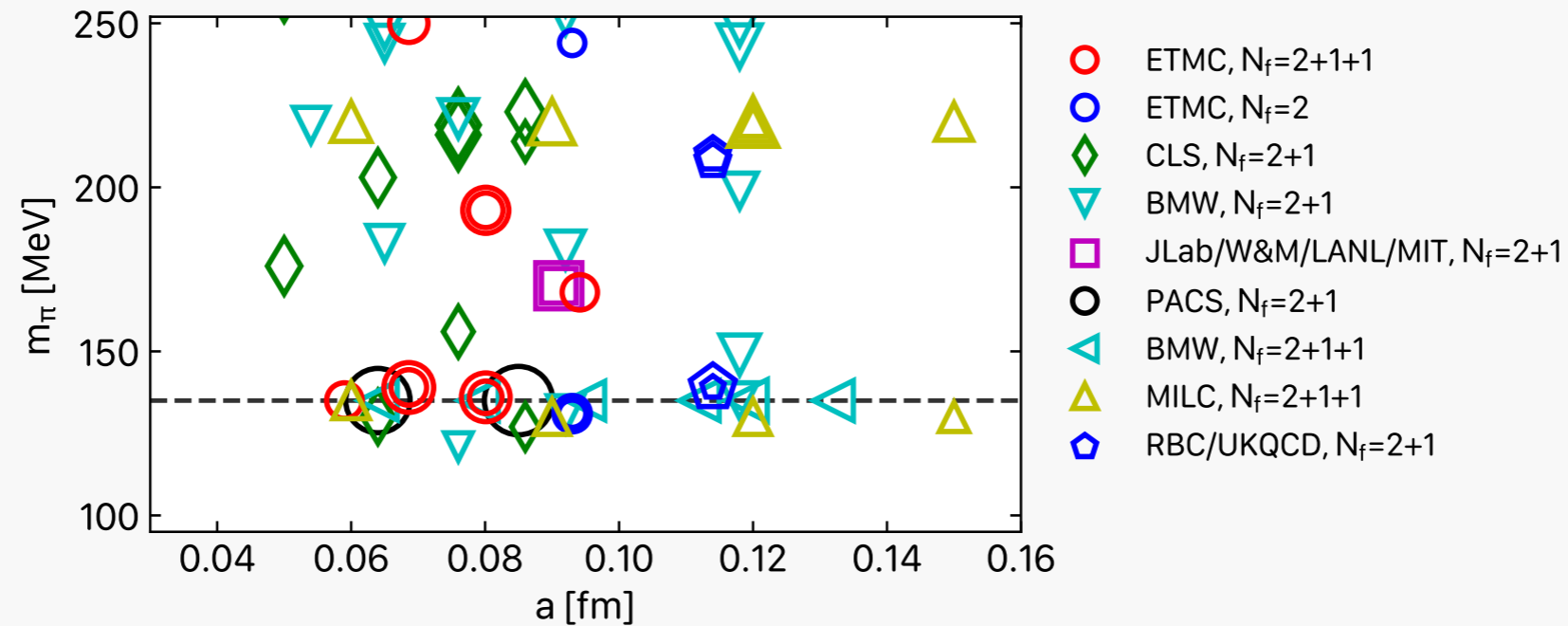
## Data analysis - post-processing

- Statistical analysis, resampling
- Statistical and stochastic errors
- Continuum and infinite volume extrapolation



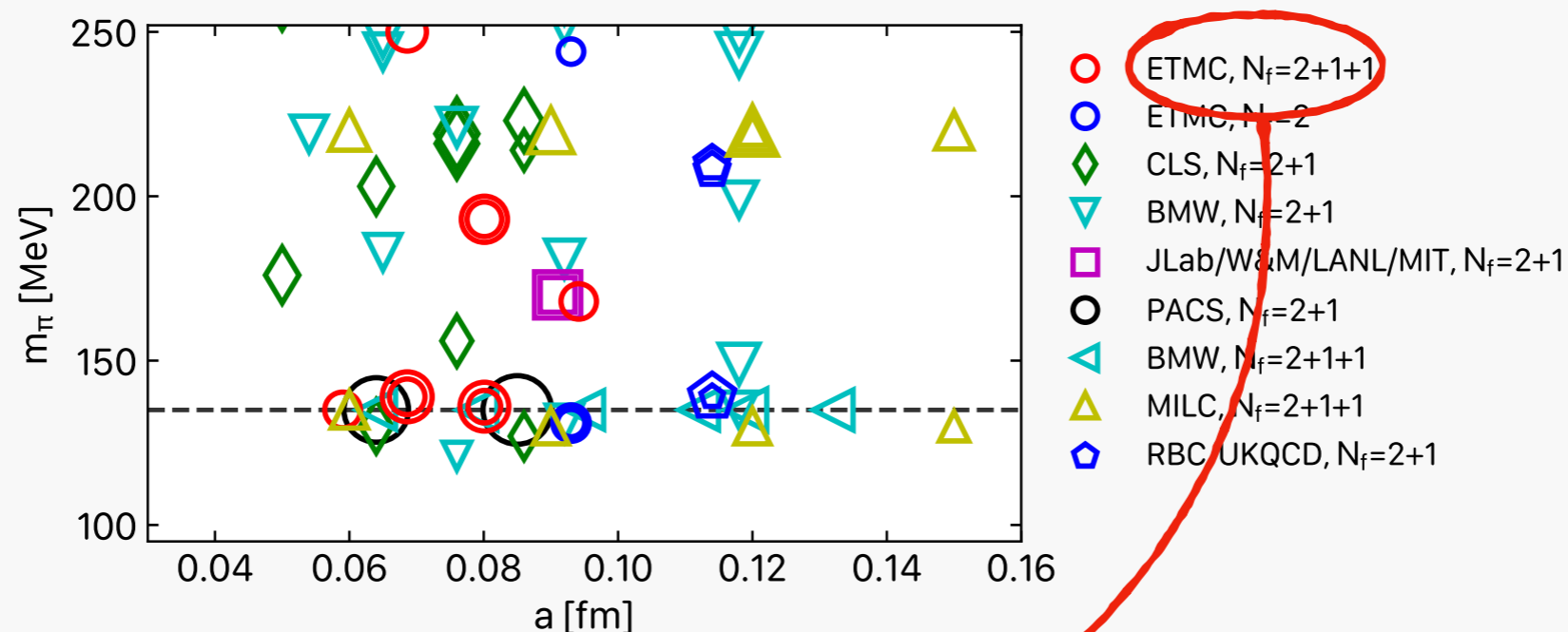
# Ensembles

Landscape of ensembles used for nucleon structure



# Ensembles

Landscape of ensembles used for nucleon structure



ETMC: three  $N_f=2+1+1$  ensembles at physical pion mass

Ens. ID (abbrv.)	Vol.	$a$ [fm]
cB211.072.64 (cB64)	$64 \times 128$	0.080
cC211.060.80 (cC80)	$80 \times 160$	0.068
cD211.054.96 (cD96)	$96 \times 192$	0.057

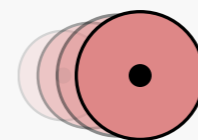
- Three lattice spacings at physical point
- Ongoing generation of finer ensembles and larger volumes
- **This talk:** 3 ensembles with:  
 $a = 0.057 - 0.08$  fm

# Local matrix elements

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

## Unpolarised

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



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

## Helicity

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



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

## Transverse

$$\mathcal{O}_{\text{T}}^{\nu\mu\mu_1\mu_2\dots\mu_n} = \bar{\psi} \sigma^{\nu} iD^{\mu_1} iD^{\mu_2} \dots iD^{\mu_n} \psi$$



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

Renormalization of lattice operators for proper continuum limit:  $\mathcal{O} = Z_{\mathcal{O}} \mathcal{O}^{\text{lat}}$

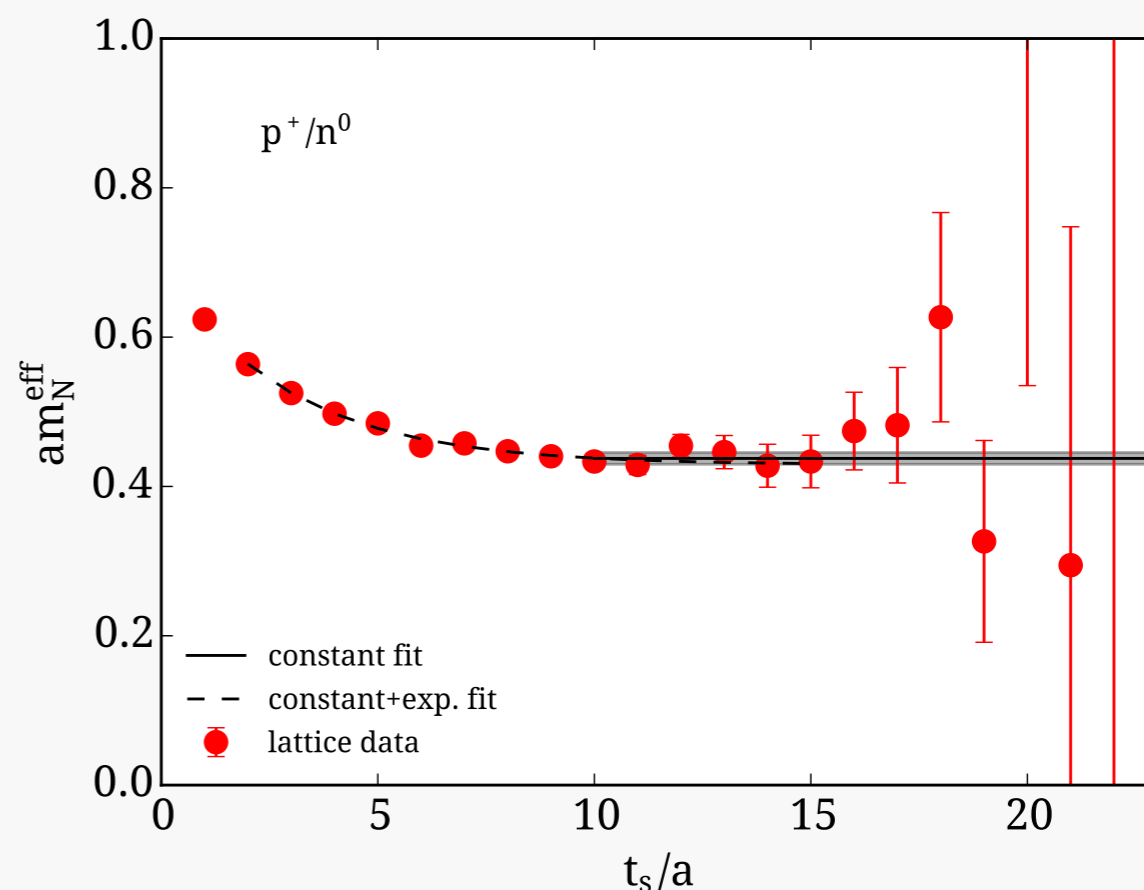
- In general,  $Z$  determined non-perturbatively in e.g. RI'-MOM scheme, converted to  $\overline{\text{MS}}$  at 2 GeV [ETM, Phys. Rev. D104 (2021) 7, 074515 [2104.13408](#)]
- $Z_A$  also available via a hadronic scheme [ETM, Phys. Rev. D107 (2023) 7, 074506 [2206.15084](#)]
- $\mathcal{O}_V$  also available via a lattice conserved current



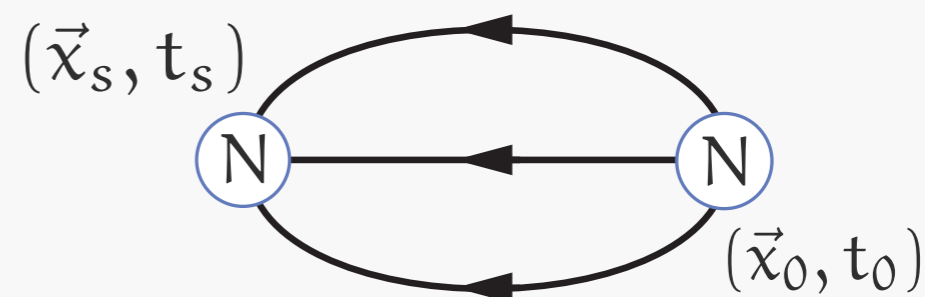
# Nucleon structure on the lattice

## Two-point correlation functions

- **Statistical error:**  $N^{-1/2}$  with Monte Carlo samples
- Correlation functions exponentially decay with time-separation
- Contamination from higher energy states



$$\sum_{\vec{x}_s} \Gamma^{\alpha\beta} \langle \bar{\chi}_N^\beta(x_s) | \chi_N^\alpha(0) \rangle = c_0 e^{-E_0 t_s} + c_1 e^{-E_1 t_s} + \dots$$



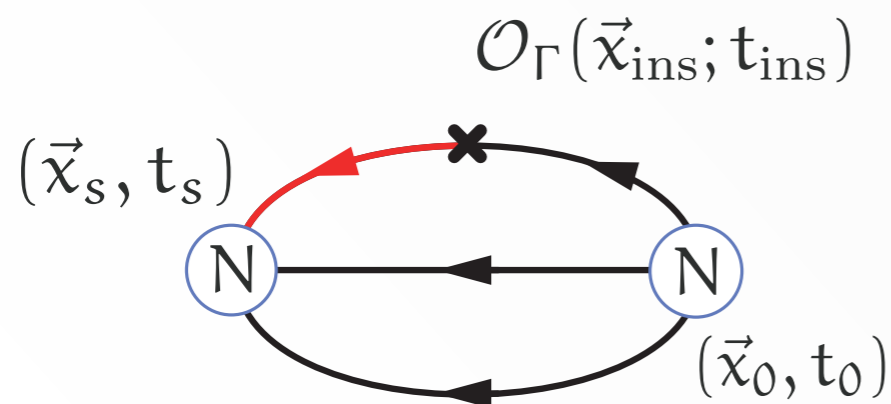
# Matrix elements on the Lattice

General three-point function:

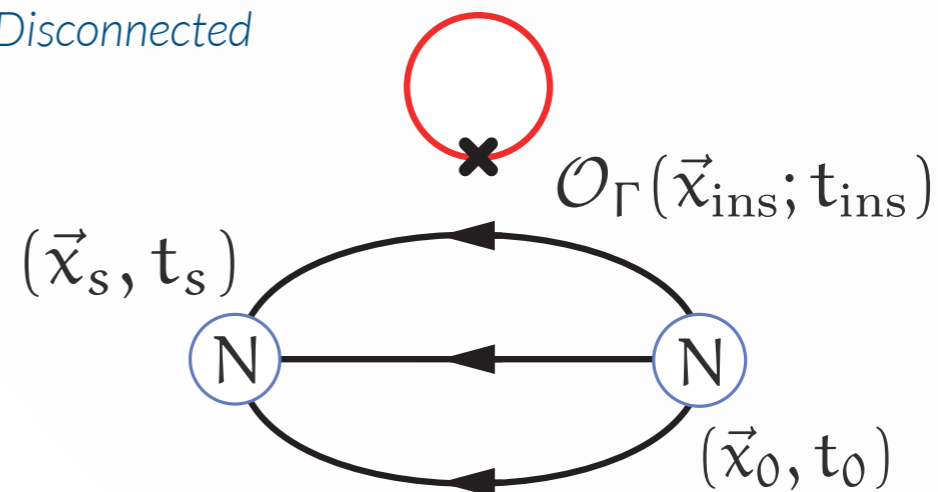
$$G_{\Gamma}(P; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s, \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} p^{\alpha\beta} \langle \bar{\chi}_{\text{N}}^{\beta}(\vec{x}_s; t_s) | \mathcal{O}_{\Gamma}(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_{\text{N}}^{\alpha}(\vec{0}; 0) \rangle$$

At quark level gives rise to both so-called connected and disconnected contributions

*Connected*



*Disconnected*



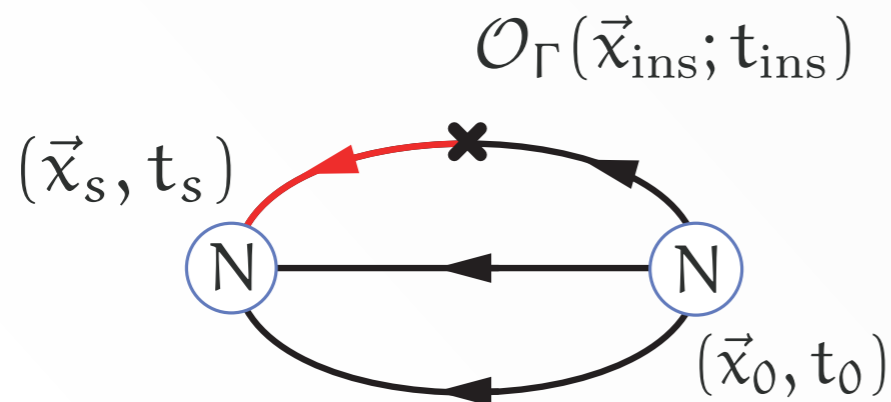
# Matrix elements on the Lattice

General three-point function:

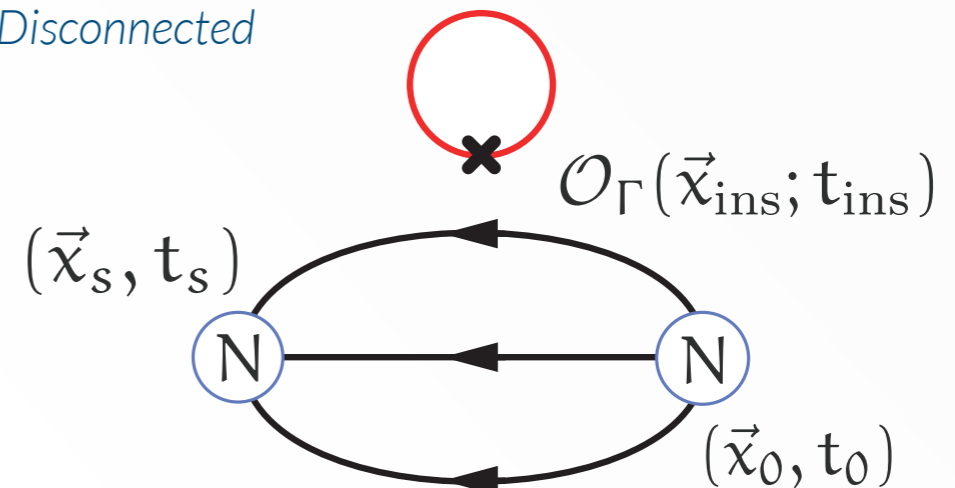
$$G_{\Gamma}(P; \vec{q}; t_s, t_{\text{ins}}) = \sum_{\vec{x}_s, \vec{x}_{\text{ins}}} e^{-i\vec{q} \cdot \vec{x}_{\text{ins}}} p^{\alpha\beta} \langle \bar{\chi}_{\text{N}}^{\beta}(\vec{x}_s; t_s) | \mathcal{O}_{\Gamma}(\vec{x}_{\text{ins}}; t_{\text{ins}}) | \chi_{\text{N}}^{\alpha}(\vec{0}; 0) \rangle$$

At quark level gives rise to both so-called connected and disconnected contributions

*Connected*

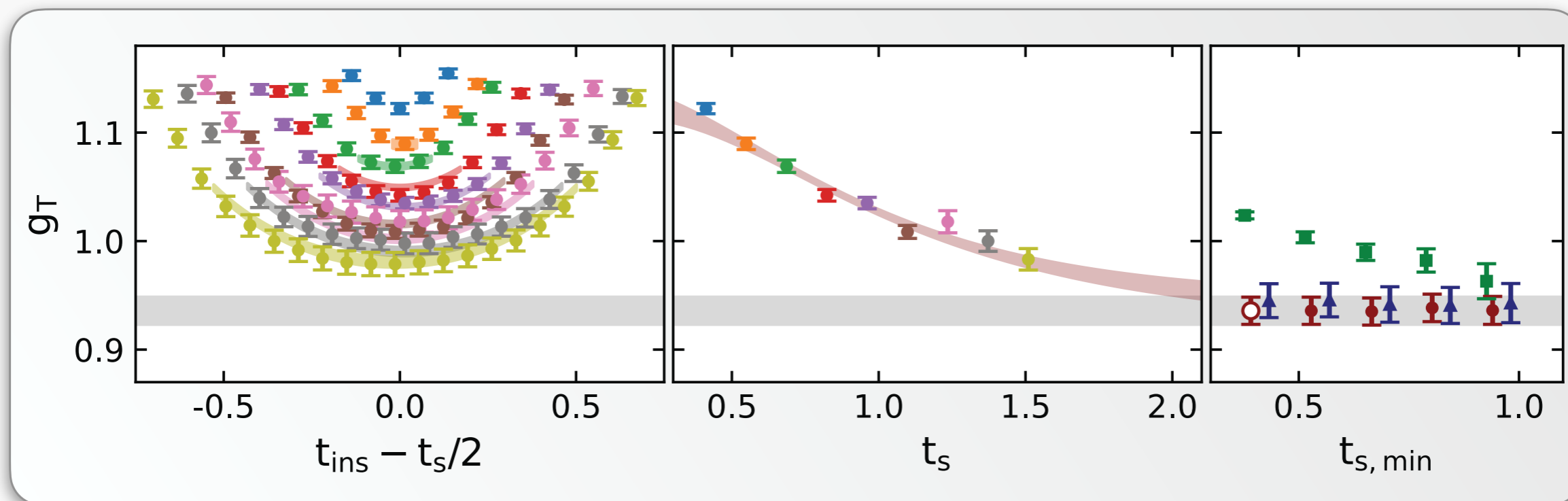


*Disconnected*



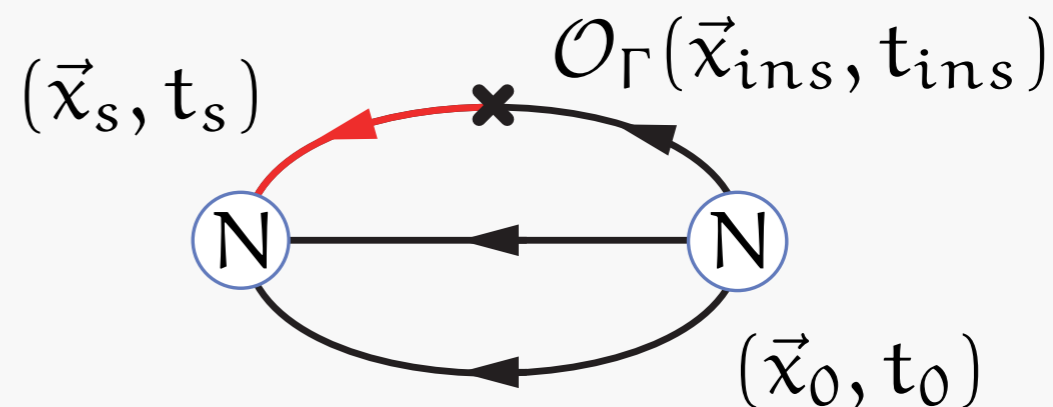
*Stochastic evaluation of loop – stochastic error in addition to statistical*

# Treatment of excited states

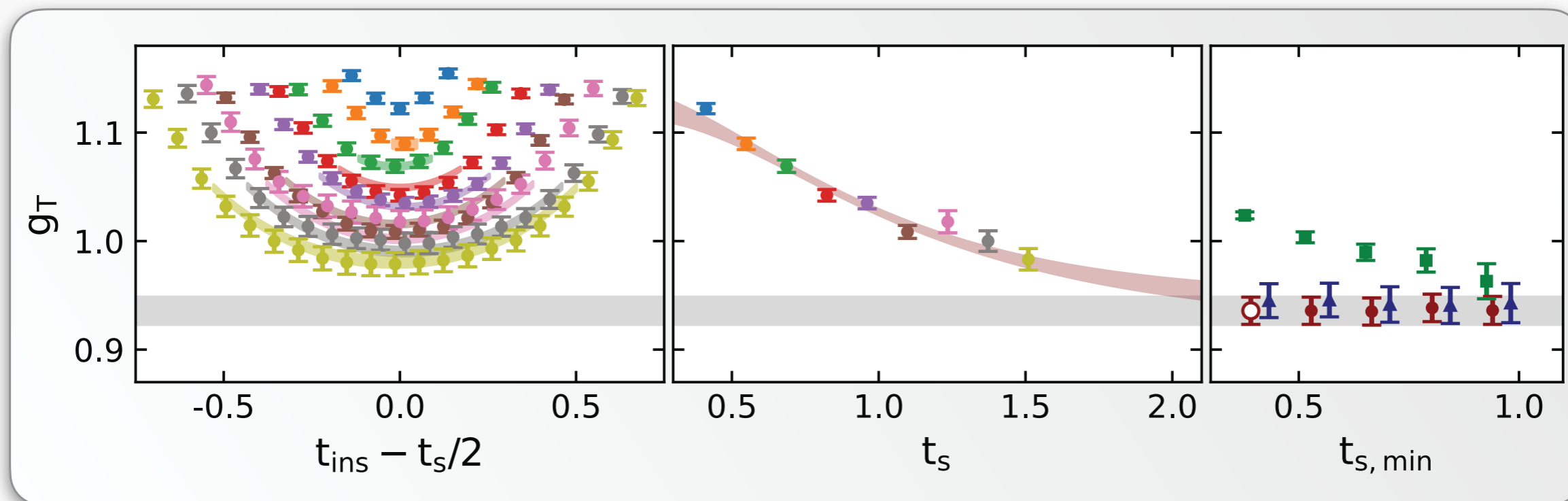


## Example from intermediate $\alpha$

- Isovector tensor charge (only connected)
- Increasing statistics with separation  $t_s$
- Summation, two- and three-state fits



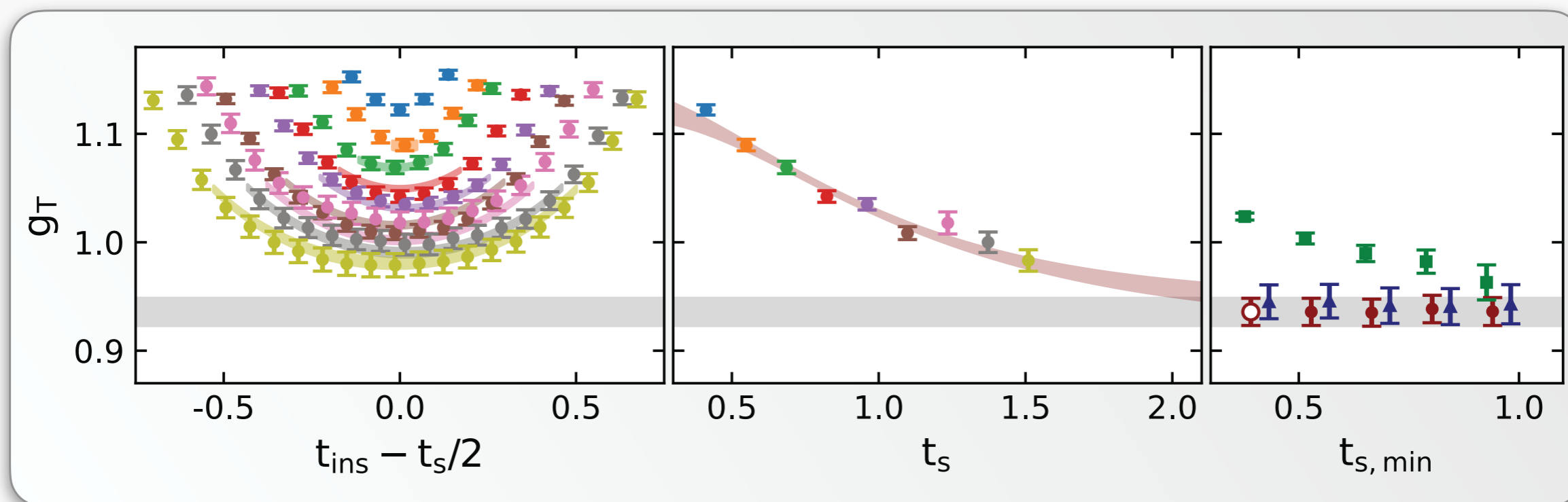
# Treatment of excited states



*Summation method*

$$S_{\Gamma}(\vec{q}; t_s) = \sum_{t_{\text{ins}}=\tau}^{t_s-\tau} R_{\Gamma}(\vec{q}; t_s; t_{\text{ins}}) \rightarrow \mathcal{M}t_s + C$$

# Treatment of excited states



Two-state fit

$$G_{\Gamma}(\vec{q}; t_s, t_{\text{ins}}) = \sum_{i=0}^1 \sum_{j=0}^1 c_{ij} e^{-E_i(0)(t_s - t_{\text{ins}})} e^{-E_j(\vec{q})t_{\text{ins}}}$$

$$\mathcal{M} = \frac{c_{00}}{\sqrt{a_0(\vec{0})a_0(\vec{q})}}$$

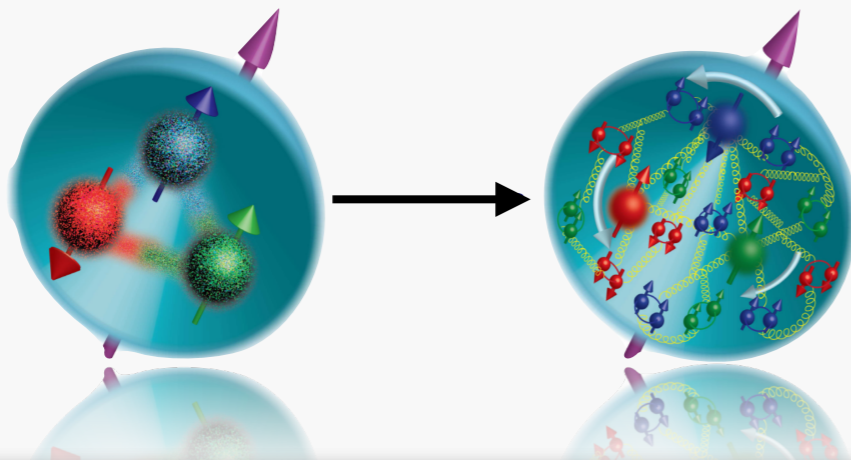
$$G(\vec{q}; t_s) = a_0(\vec{q})e^{-\varepsilon_0(\vec{q})t_s} + a_1(\vec{q})e^{-\varepsilon_1(\vec{q})t_s}$$

# Nucleon axial charge

Matrix element of the axial current

Isovector case well known from  $\beta$ -decay:  $\langle p | \bar{u} \gamma_5 \gamma_k d | n \rangle$

Flavor-separated contributions to axial charge relate to quark intrinsic spin contributions to nucleon spin

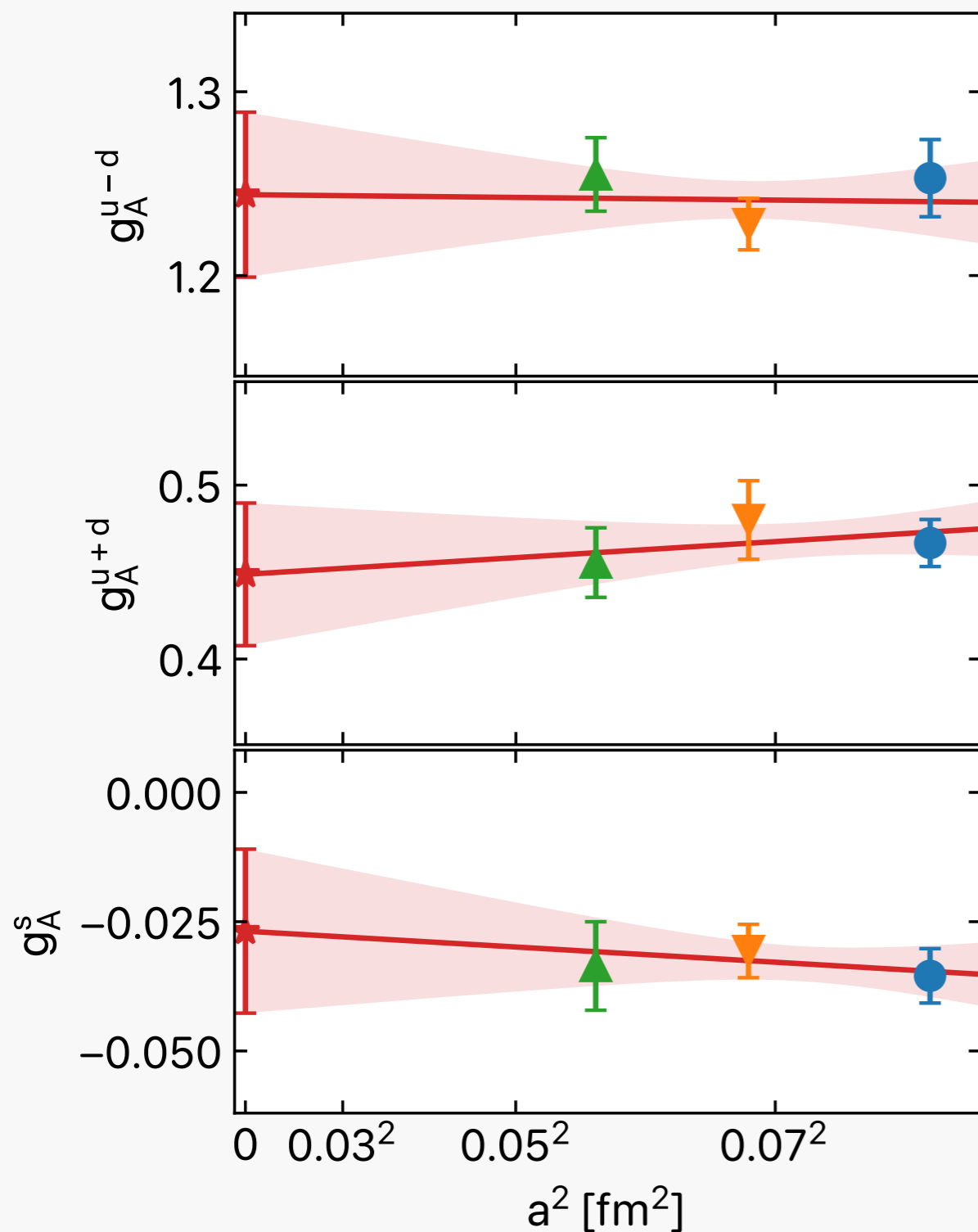


$$\frac{1}{2} \Delta \Sigma = \frac{1}{2} \sum_{q=u,d,s,\dots} g_A^q$$

## 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)

# Nucleon axial charge



Recent result by ETM collaboration;  
three values of  $a$  at physical  $m_\pi$

ETM collab., Phys. Rev. D 109 (2024) 3, 034503  
[[arXiv:2309.05774](https://arxiv.org/abs/2309.05774)]

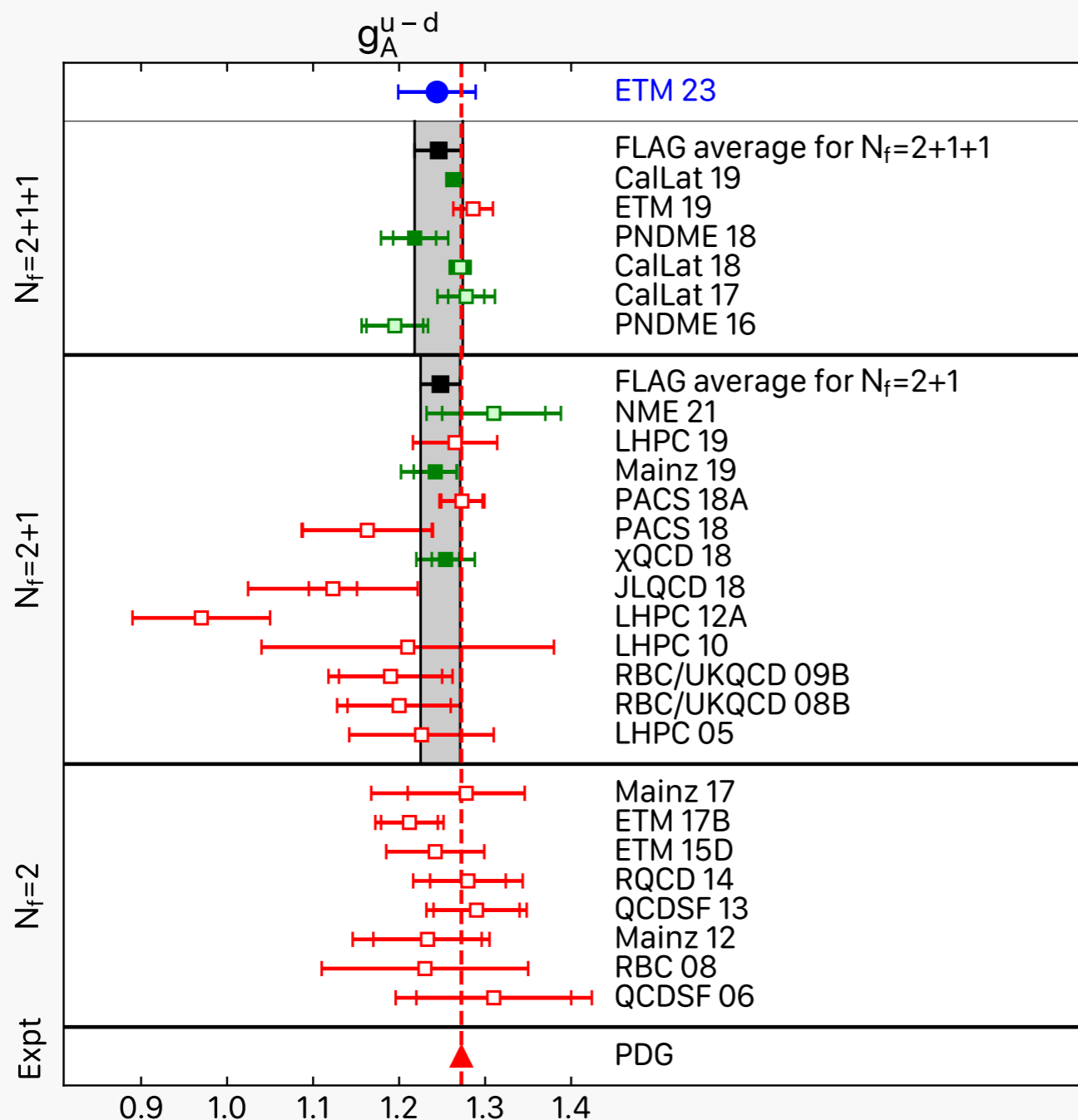
- Errors for each ensemble include *statistical* and *systematic* due to excited state contamination
- Model averaged to evaluate systematic errors due to excited state contamination (see e.g. [arXiv:2208.14983](https://arxiv.org/abs/2208.14983))

Preliminary!

Complete analysis for flavour separated charges ongoing



# Nucleon axial charge



## Latest FLAG21 values

- ETM23 consistent with FLAG average
- Agreement for  $g_A$  means confidence for more challenging quantities
- E.g.
  - Scalar ME,  $\sigma$ -terms

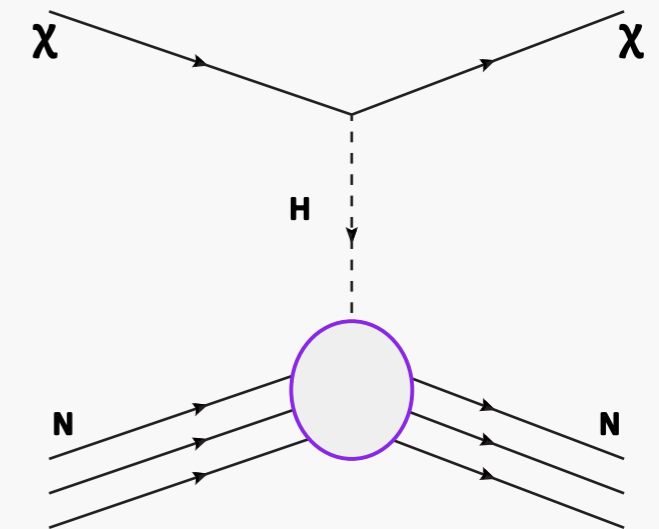
$$\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle$$

- Tensor ME

$$g_T = \langle 1 \rangle_{\delta u - \delta d} \leftarrow \langle N | \bar{u} \sigma_{\mu\nu} u + \bar{d} \sigma_{\mu\nu} d | N \rangle$$

# Scalar charge – $\sigma$ -terms

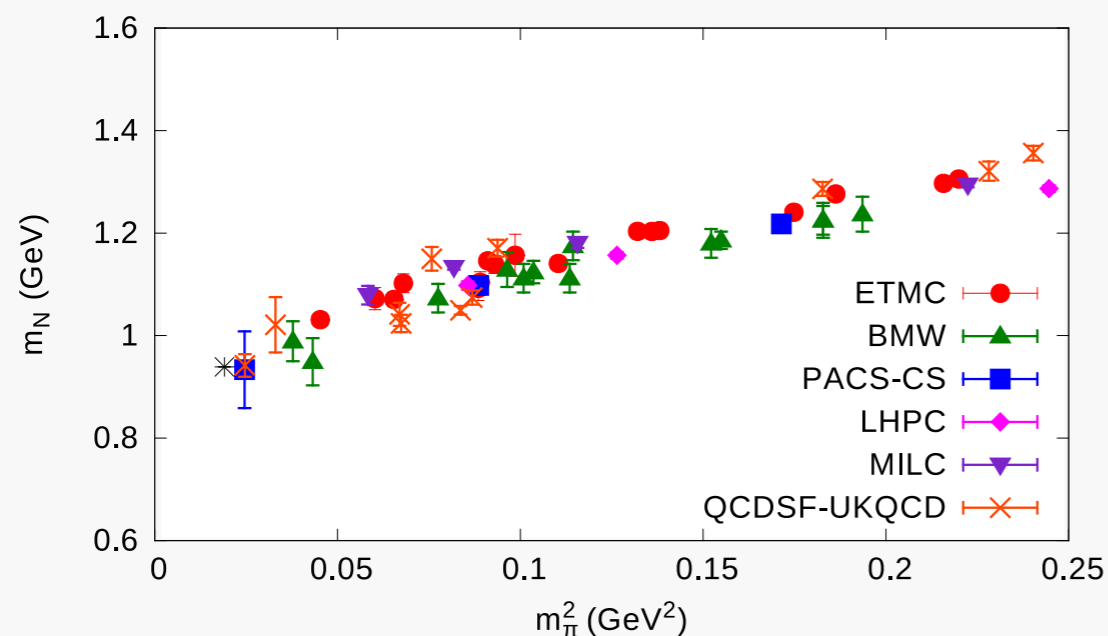
- Pion nucleon  $\sigma$ -term:  $\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle$
- Strange  $\sigma$ -term:  $\sigma_s = m_s \langle N | \bar{s}s | N \rangle$
- Enter super-symmetric candidate particle scattering cross sections with nucleon (e.g. neutralino through Higgs)



## 1. Direct calculation of matrix elements

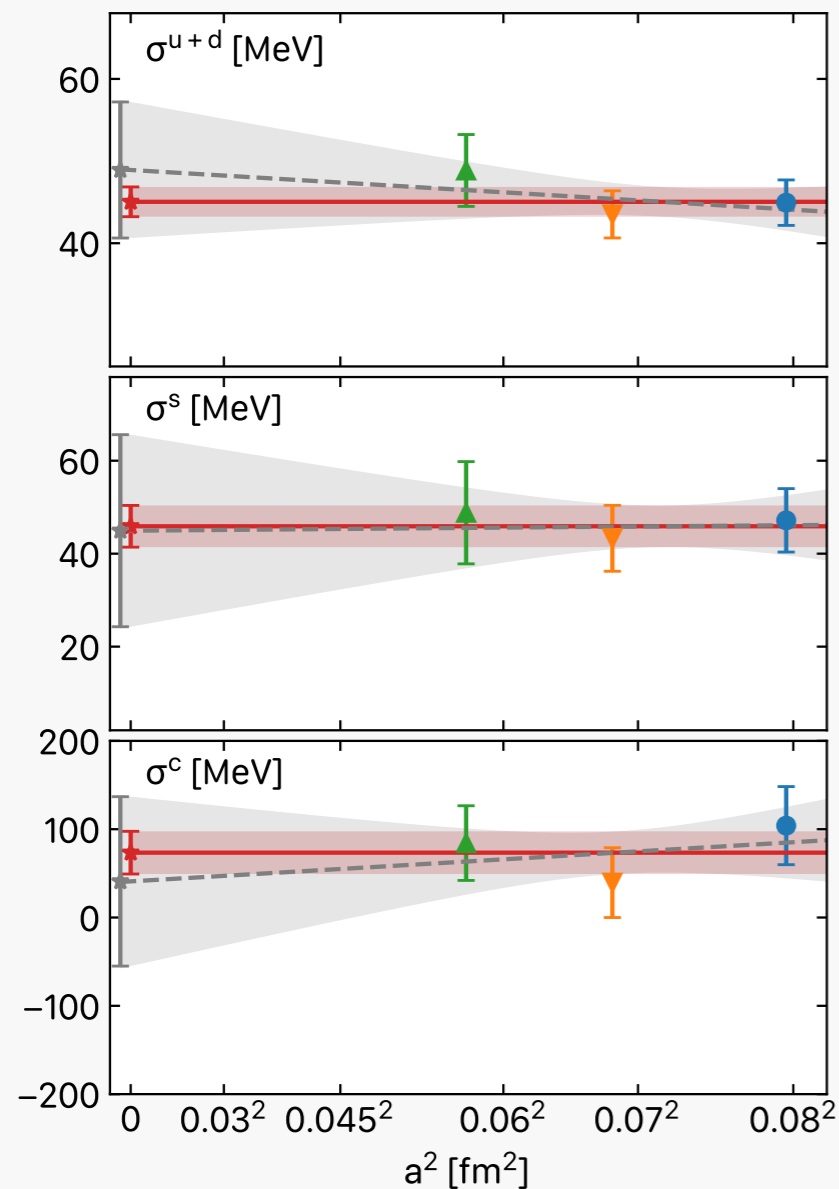
Involves disconnected contributions

## 2. Through Feynman - Hellmann theorem: $\sigma_{\pi N} = m_{ud} \frac{\partial m_N}{\partial m_{ud}}$ $\sigma_s = m_s \frac{\partial m_N}{\partial m_s}$

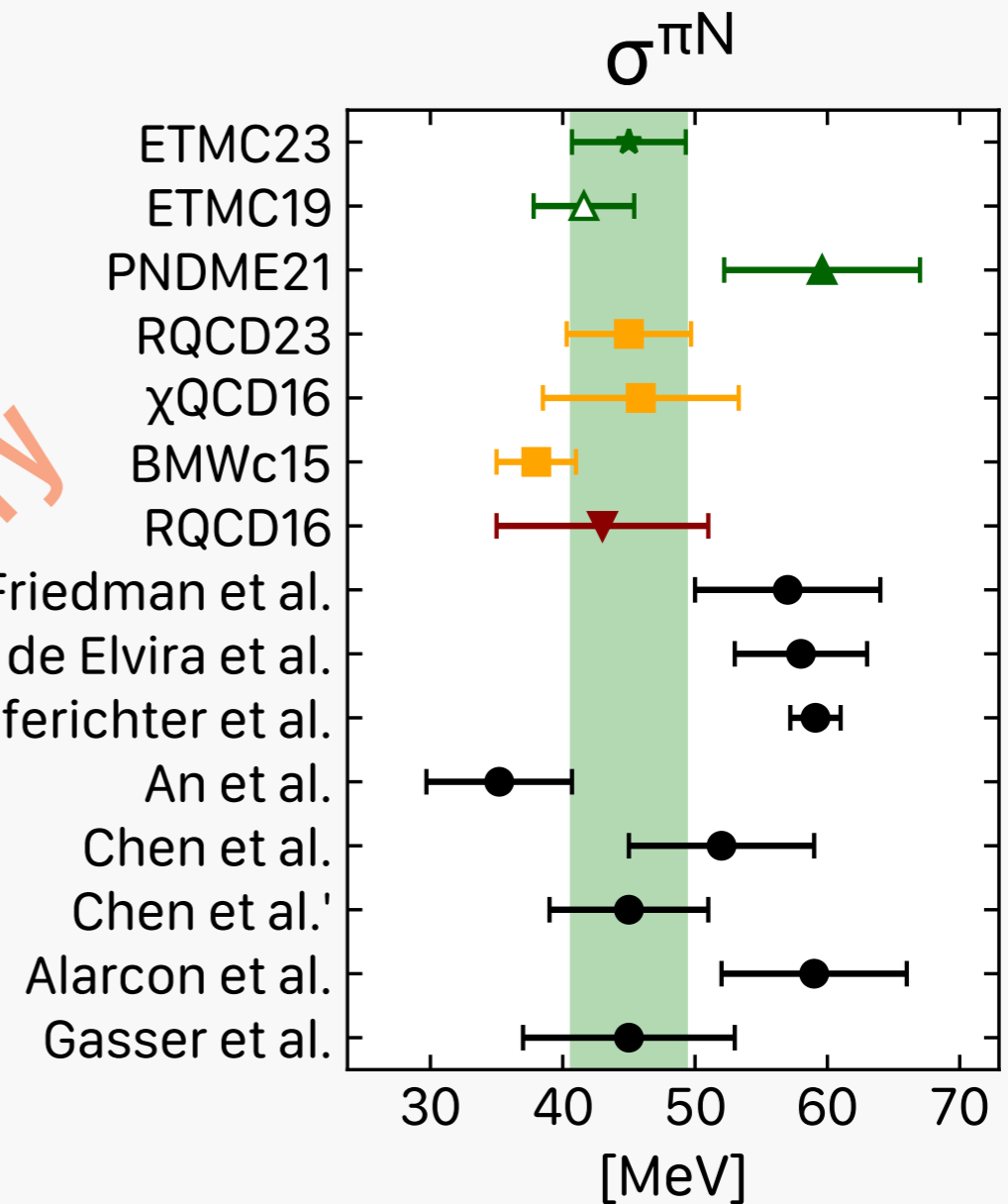


- Reliance on effective theories for dependence on  $m_\pi$
- Weak dependence on  $m_s$

# Scalar charge – $\sigma$ -terms

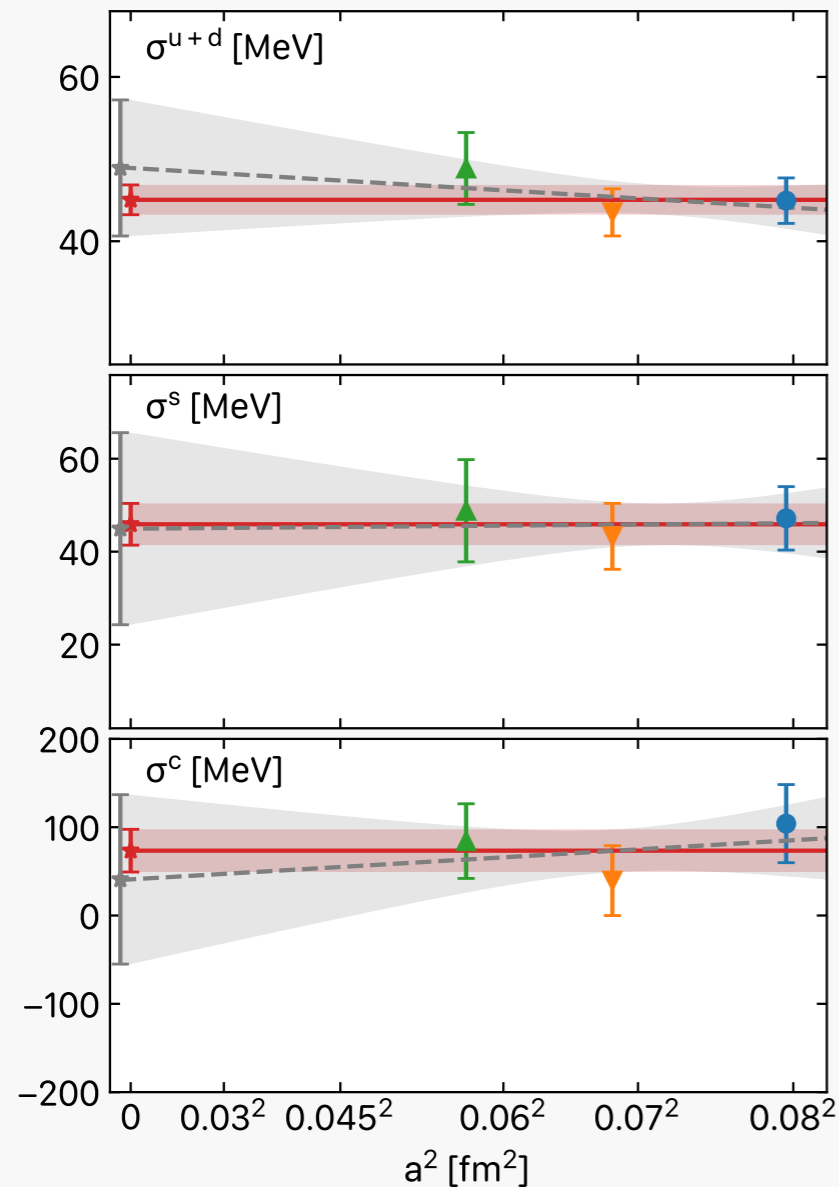


Preliminary

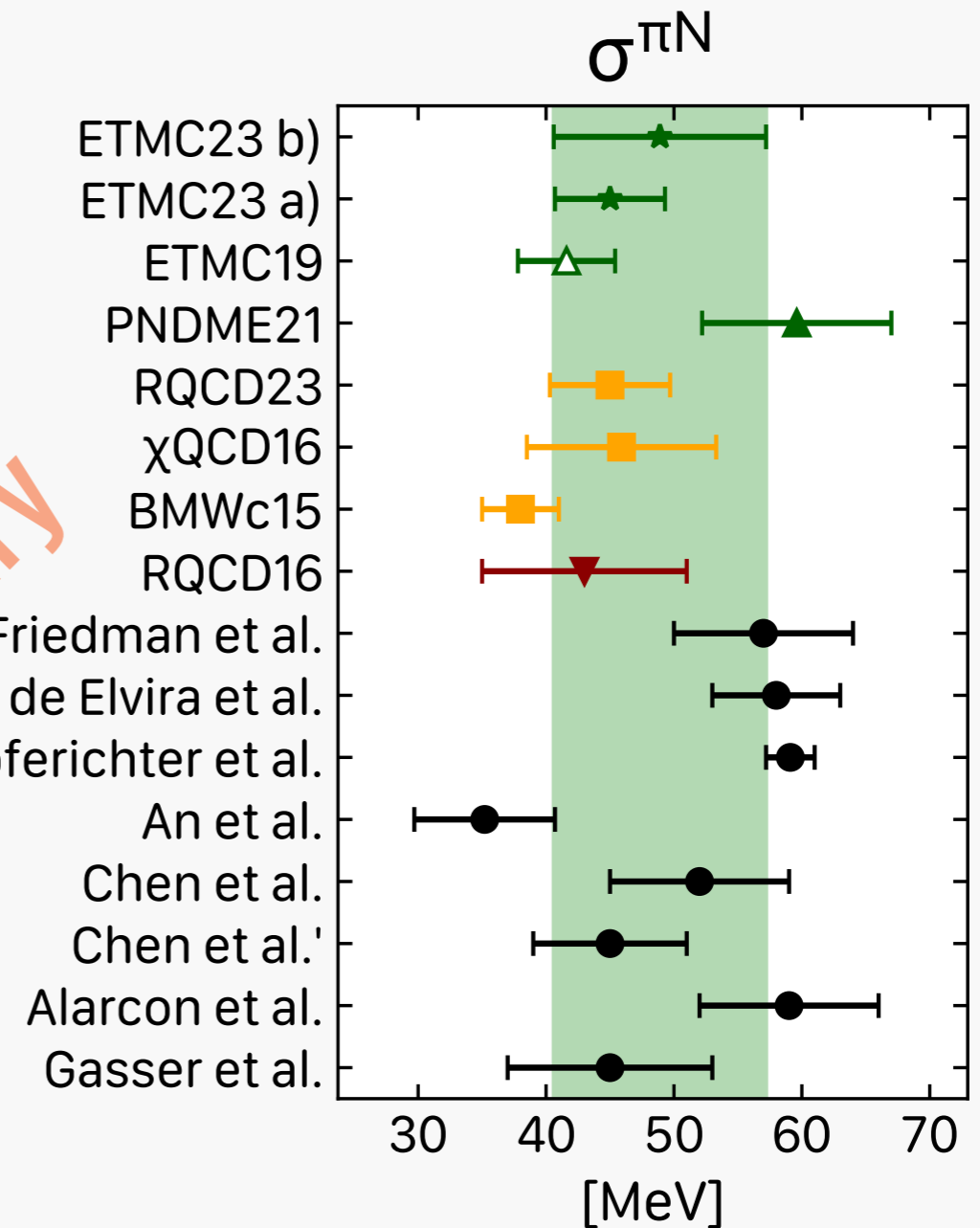


- One result using FH method (BMW)
- Los Alamos group [R. Gupta et al. PRL 127 (2021) 24]:  
 →  $59.6(7.4)$  MeV, with explicit  $\pi N$  as prior

# Scalar charge – $\sigma$ -terms

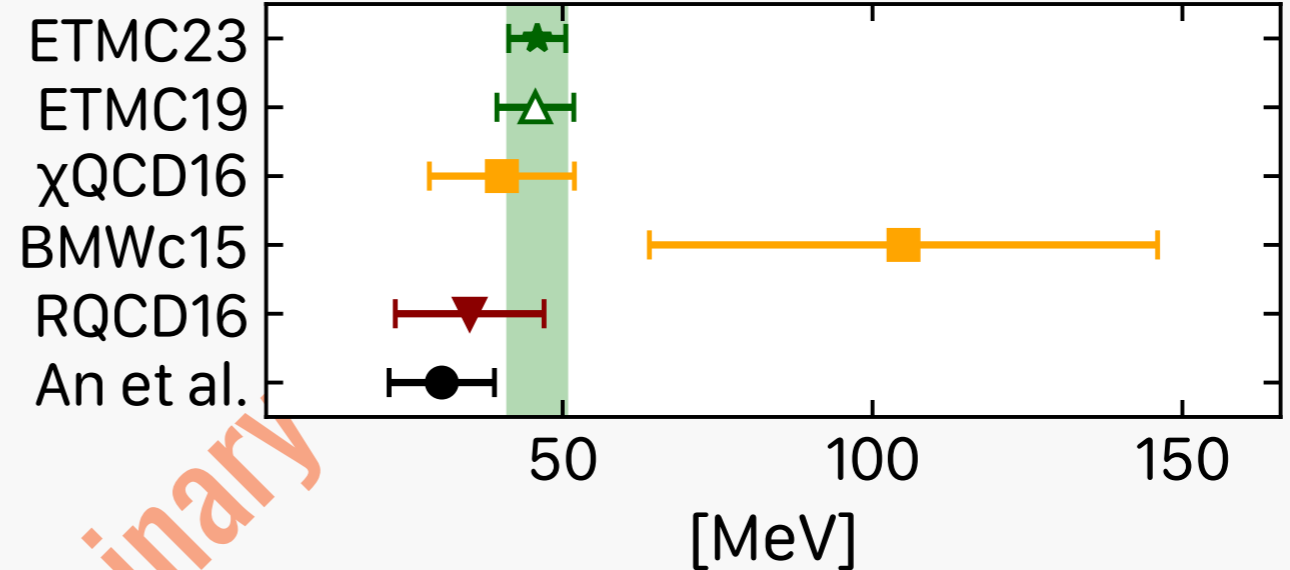
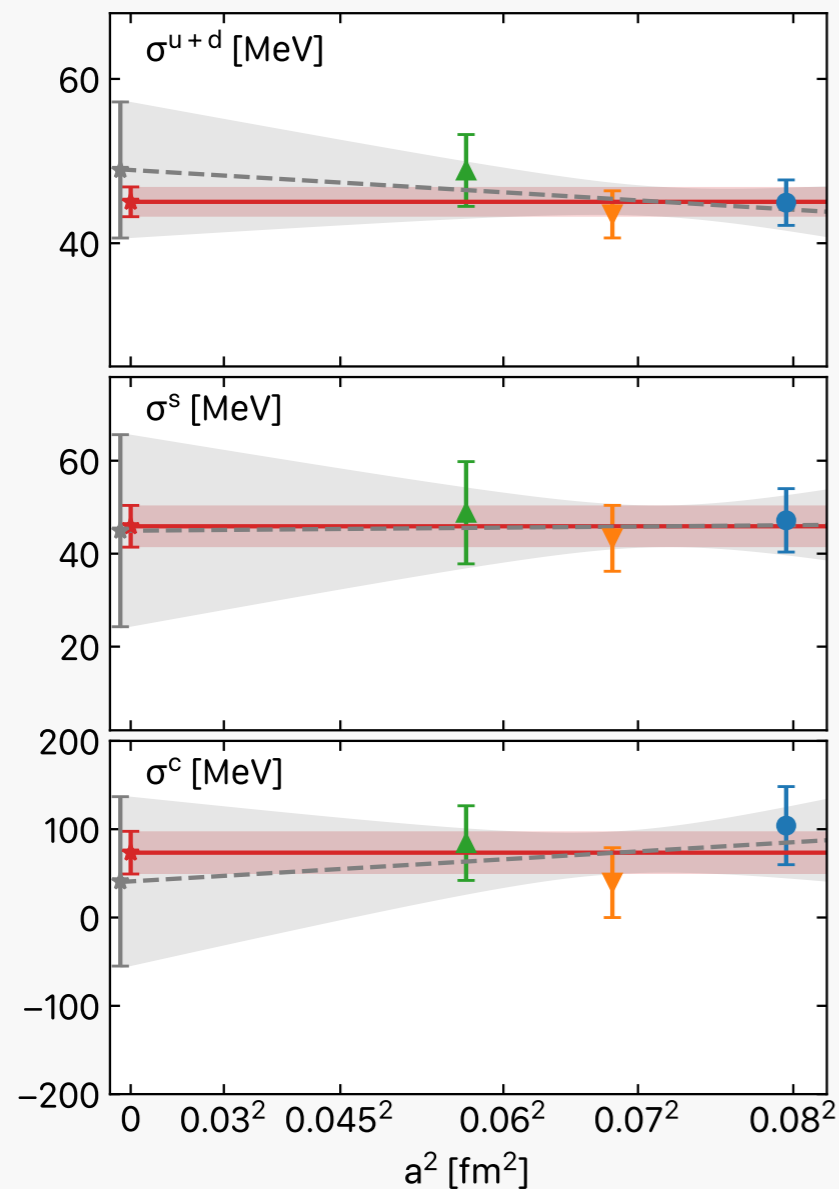


Preliminary



- One result using FH method (BMW)
- Los Alamos group: 59.6(7.4) MeV, when explicitly including  $\pi N$  energy as prior
- Our result with linear continuum extrapolation (Grey band in left plot)

# Scalar charge – $\sigma$ -terms



Preliminary

## Strange content of the nucleon

- Weaker dependence on lattice spacing
- Overall general agreement between lattice formulations

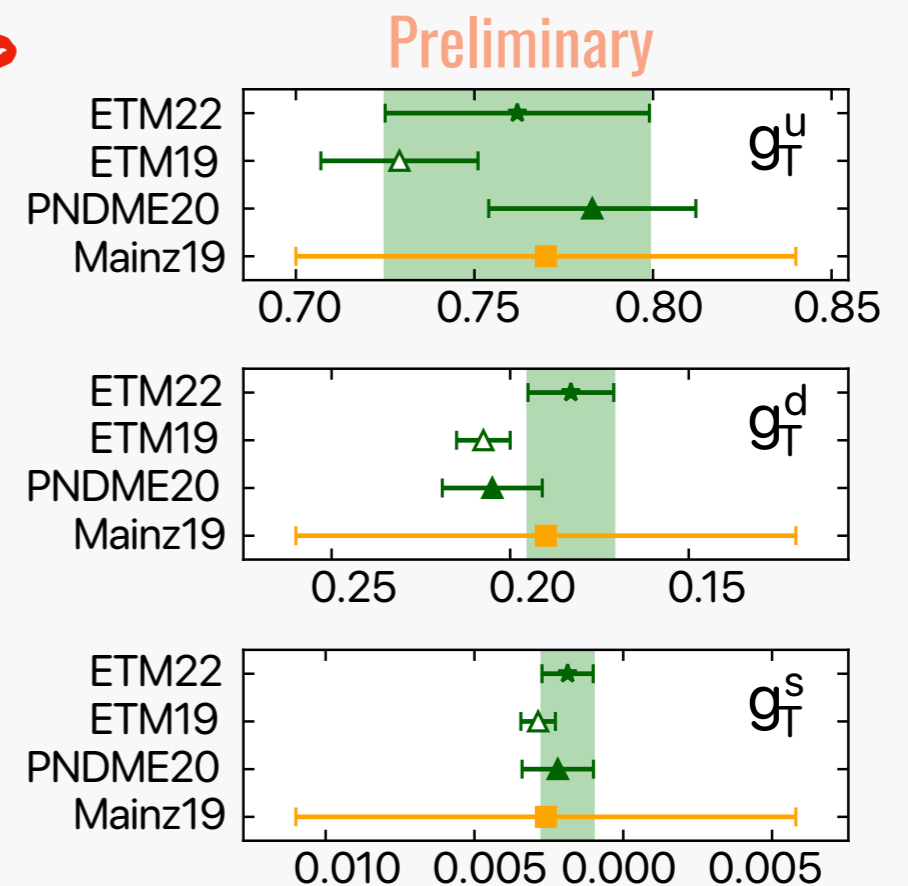
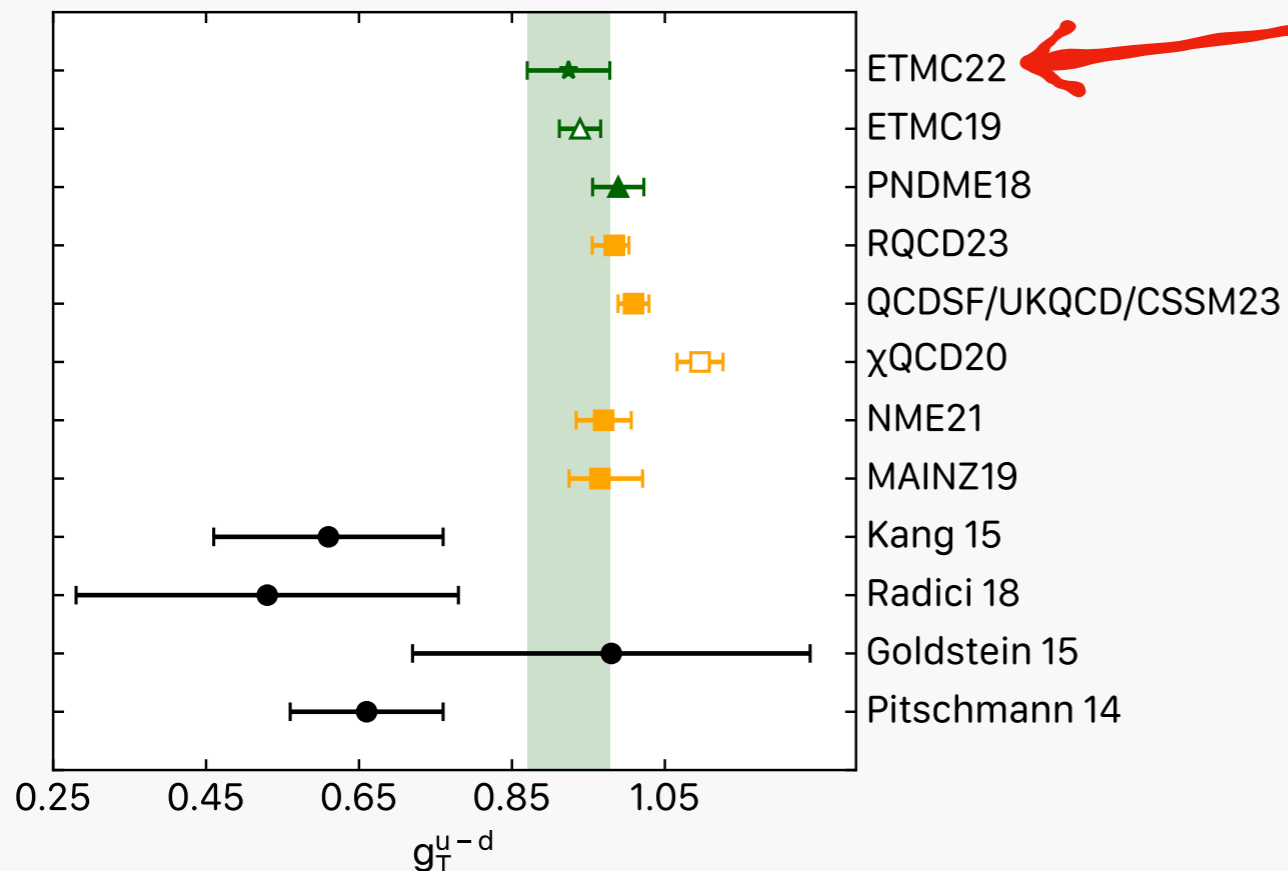
# Tensor charge

- Tensor matrix element

$$g_T = \langle 1 \rangle_{\delta q} \leftarrow \langle N | \bar{q} \sigma_{\mu\nu} q | N \rangle \quad \delta q \in \{ \delta u + \delta d, \delta u - \delta d, \delta s, \dots \}$$

- Novel CP-violating interactions, non-zero nEDM
- Moment of transversity PDF; Can be used to constrain experimental analyses, e.g. JAM [Phys. Rev. D 106 (2022) 3, 034014 [arXiv:2205.00999](https://arxiv.org/abs/2205.00999)]

“First moments of the nucleon transverse quark spin densities using lattice QCD”, Phys. Rev. D107 (2023) 5, 054504 [[arXiv:2202.09871](https://arxiv.org/abs/2202.09871)]



# Nucleon Electromagnetic Form Factors

Matrix element:

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

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

**Dirac and Pauli ( $F_1$  and  $F_2$ ) / Sachs Electric and Magnetic ( $G_E$  and  $G_M$ ) form-factors:**

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

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

**Isovector & Isoscalar currents:**

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

$$j_\mu^s = \bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d$$

Assuming mass  
degenerate up and  
down quarks

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

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

# Treatment of excited states

Summation method

$$S_{\Gamma}(\vec{q}; t_s) = \sum_{t_{\text{ins}}=\tau}^{t_s-\tau} R_{\Gamma}(\vec{q}; t_s; t_{\text{ins}}) \rightarrow \mathcal{M}t_s + C$$

Two-state fit

$$G_{\Gamma}(\vec{q}; t_s, t_{\text{ins}}) = \sum_{i=0}^1 \sum_{j=0}^1 c_{ij} e^{-E_i(0)(t_s-t_{\text{ins}})} e^{-E_j(\vec{q})t_{\text{ins}}}$$

$$\mathcal{M} = \frac{c_{00}}{\sqrt{a_0(\vec{0})a_0(\vec{q})}}$$

$$G(\vec{q}; t_s) = a_0(\vec{q})e^{-\varepsilon_0(\vec{q})t_s} + a_1(\vec{q})e^{-\varepsilon_1(\vec{q})t_s}$$

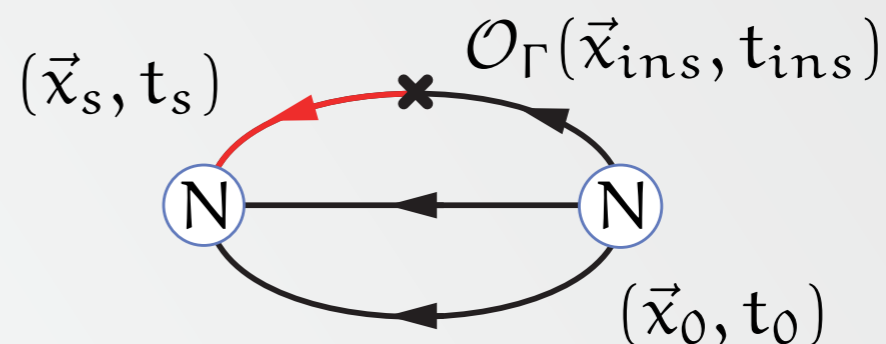
Ground state:

$$E_0(0) = \varepsilon_0(0)$$

$$E_0(\vec{q}) = \varepsilon_0(\vec{q}) = [\varepsilon_0^2(\vec{0}) + (\frac{2\pi}{L}\vec{q})^2]^{\frac{1}{2}}$$

Excited states:

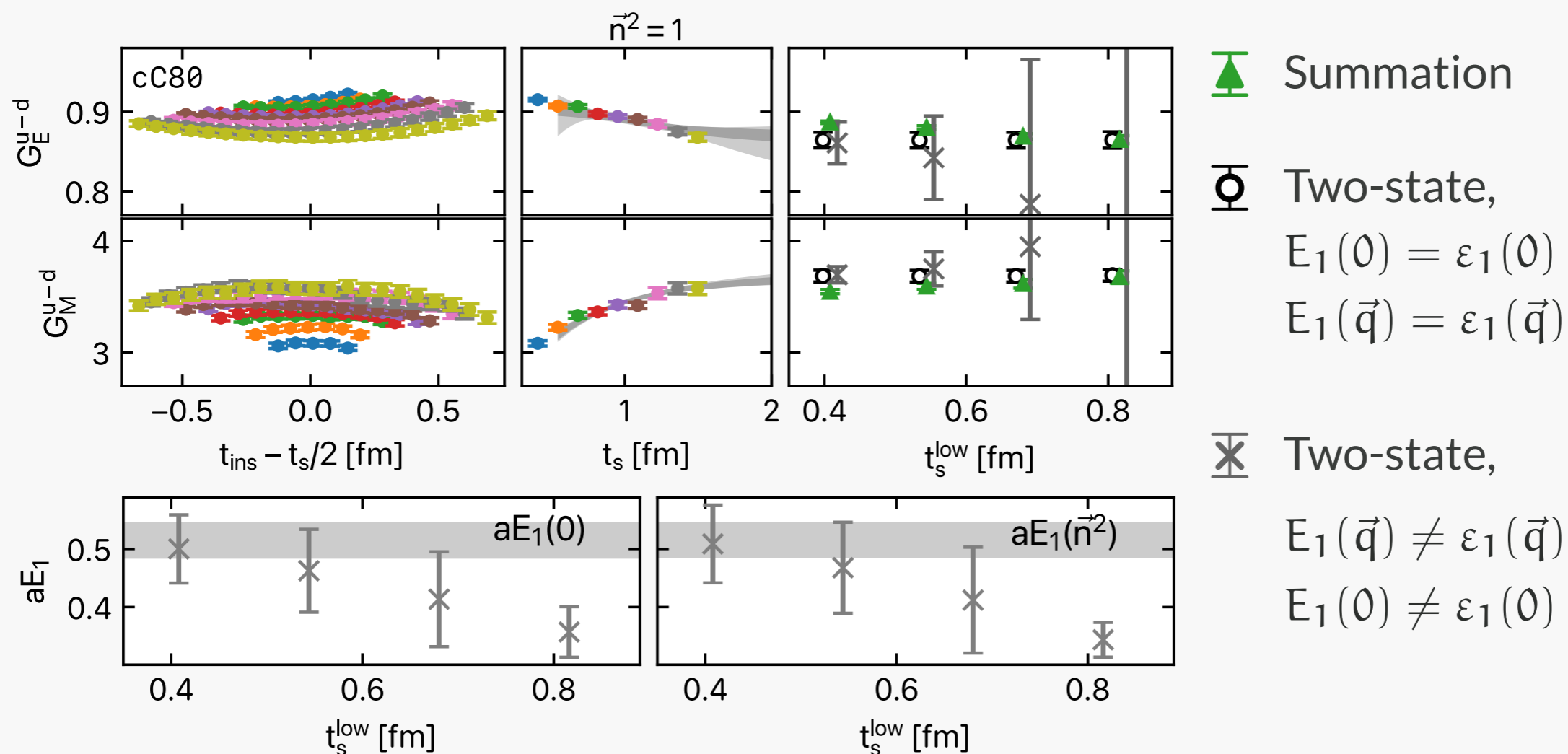
In general,  $E_1(\vec{q}) \neq \varepsilon_1(\vec{q})$  and  $E_1(0) \neq \varepsilon_1(0)^*$



\*E.g. arXiv:1905.06470

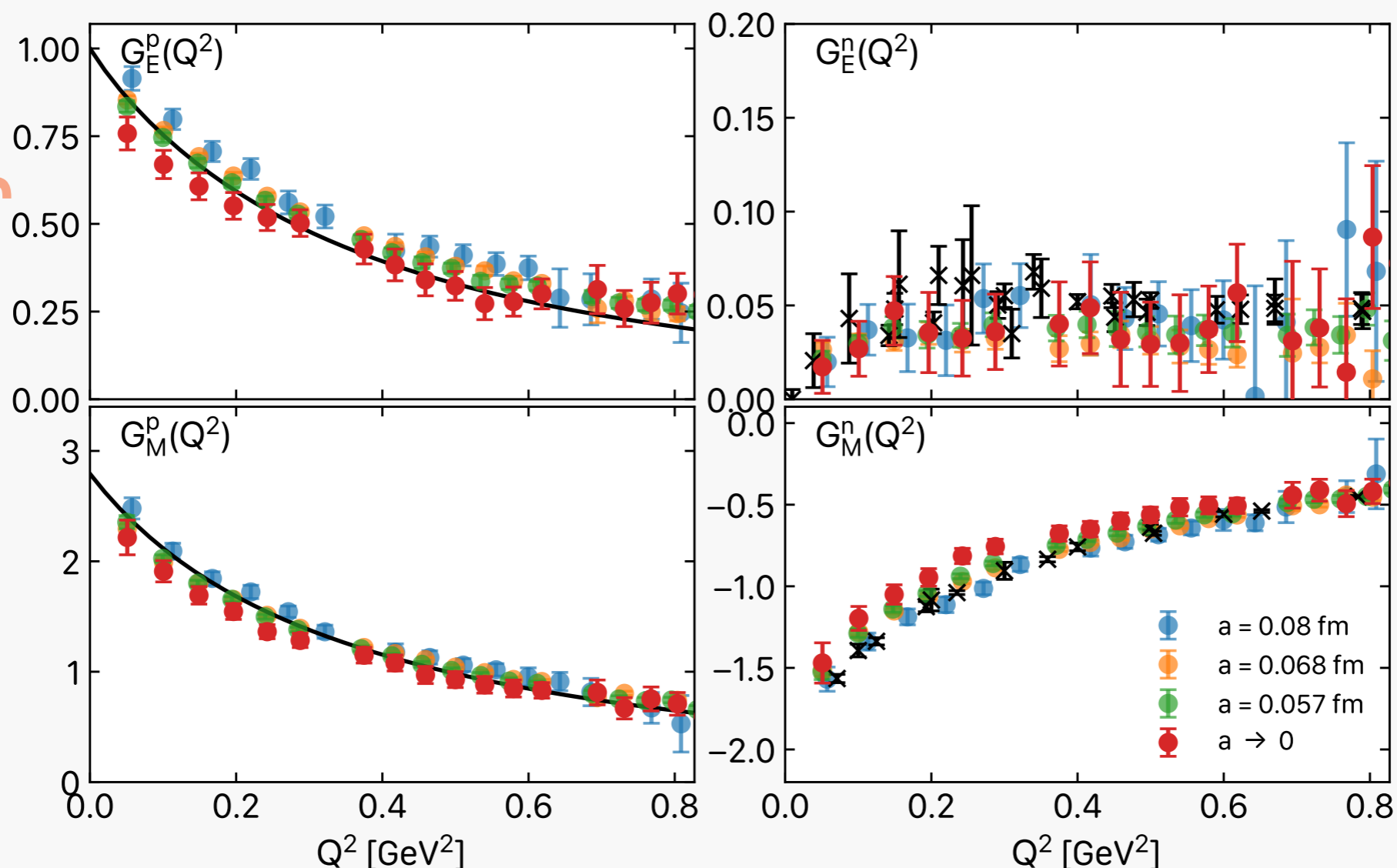


# Treatment of excited states



# Proton & neutron form factors

Preliminary



- Includes disconnected for  $u+d$  combination
- Black curve for proton  $\rightarrow$  from  $z$ -expansion fits to world data (experiment)
- Black crosses for neutron  $\rightarrow$  world data (experiment)
- Ongoing analysis for proton and neutron radii, magnetic moment

# Axial Form Factors

Matrix element:

$$\langle N(\mathbf{p}', s') | A_\mu^3 | N(\mathbf{p}, s) \rangle = \sqrt{\frac{M_N^2}{E_N(\mathbf{p}') E_N(\mathbf{p})}} \bar{u}(\mathbf{p}', s') \mathcal{O}^\mu u(\mathbf{p}, s)$$
$$\mathcal{O}^\mu = \gamma_\mu \gamma_5 G_A(q^2) + \frac{q^\mu \gamma_5}{2M_N} G_P(q^2), \quad q = \mathbf{p}' - \mathbf{p}$$

**Axial ( $G_A$ ) and Induced Pseudoscalar ( $G_P$ ) form factors**

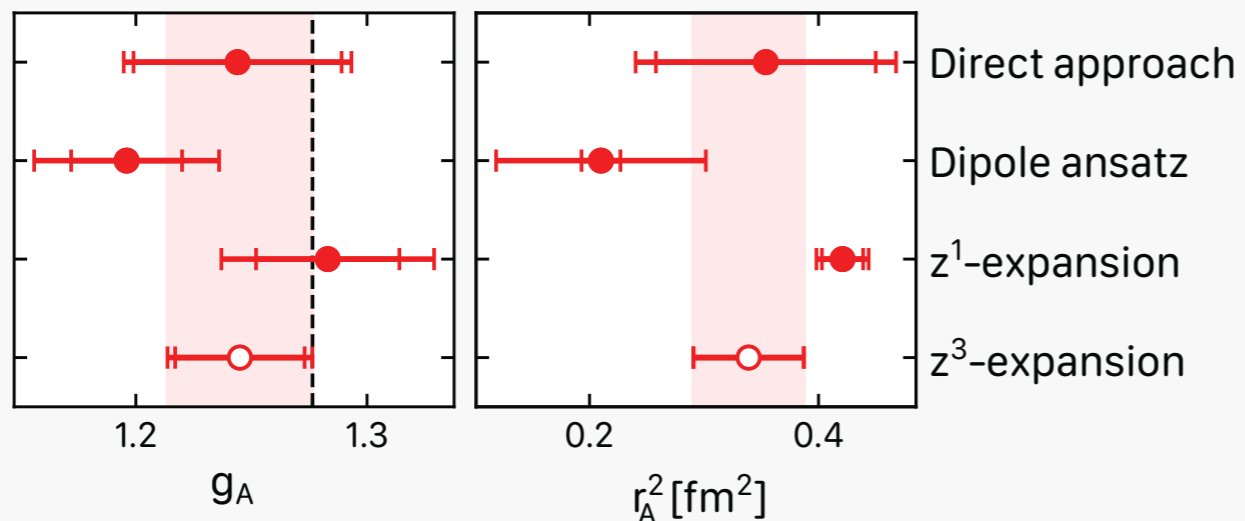
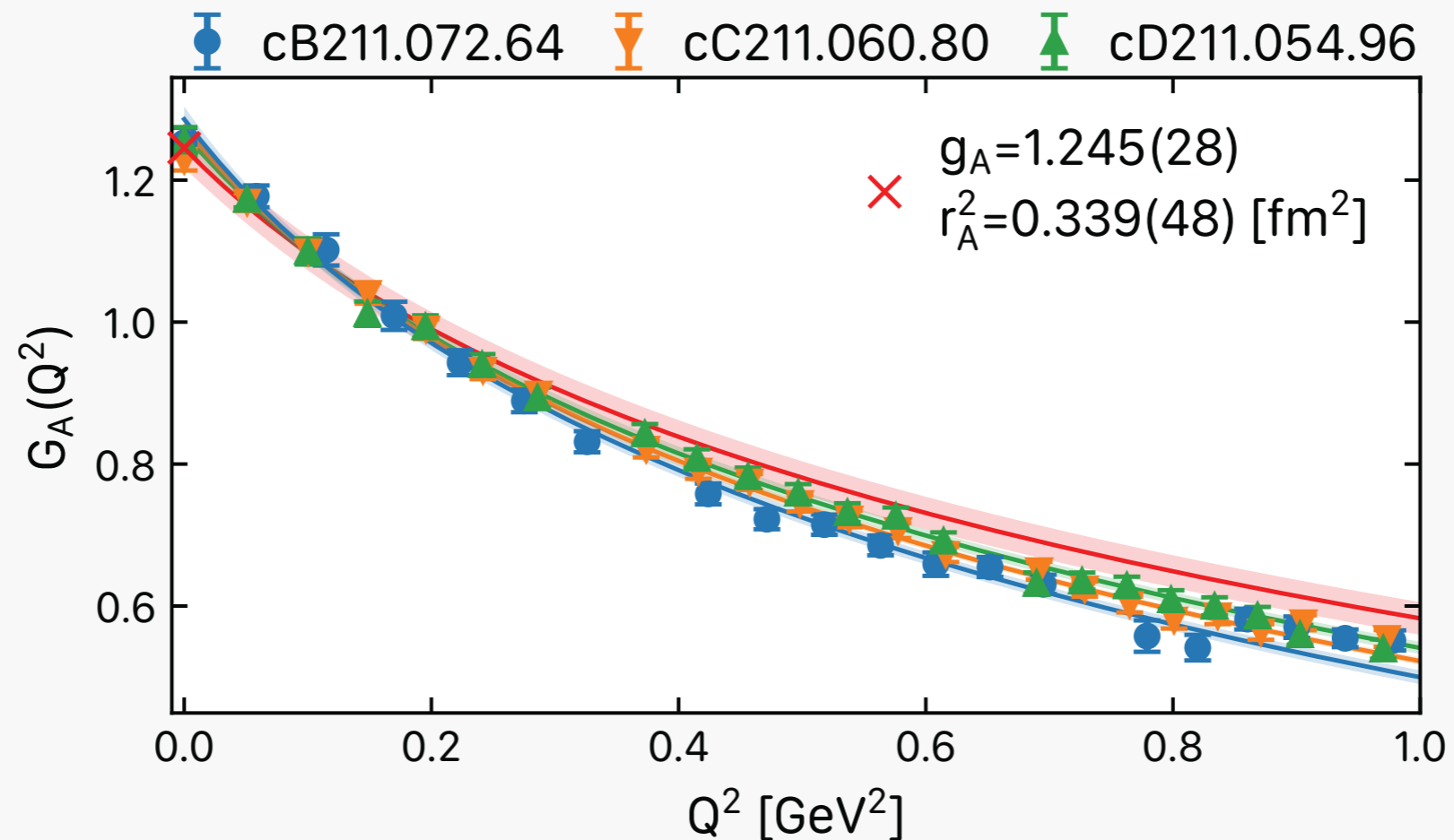
- Known to less accuracy experimentally compared to EM
  - Via elastic scattering:  $\nu_\mu + n \rightarrow \mu^- + p$
  - Via charged pion electroproduction
- Required in neutrino oscillation experiments. Traditionally modelled with a dipole form:

$$G_A(Q^2) = \frac{g_A}{(1 + Q^2/M_A^2)^2} \text{ to extract the "axial mass" } M_A$$

- Note, the lattice calculation of the isovector case:

$$\langle p(p') | \bar{u} \gamma_5 \gamma_\mu d | n(p) \rangle \xrightarrow{p \leftrightarrow n} \langle N(p') | \bar{u} \gamma_5 \gamma_\mu u - \bar{d} \gamma_5 \gamma_\mu d | N(p) \rangle$$

# Axial Form Factor



- Nice agreement of results independent of fit
- Compare to experiment (dashed line)

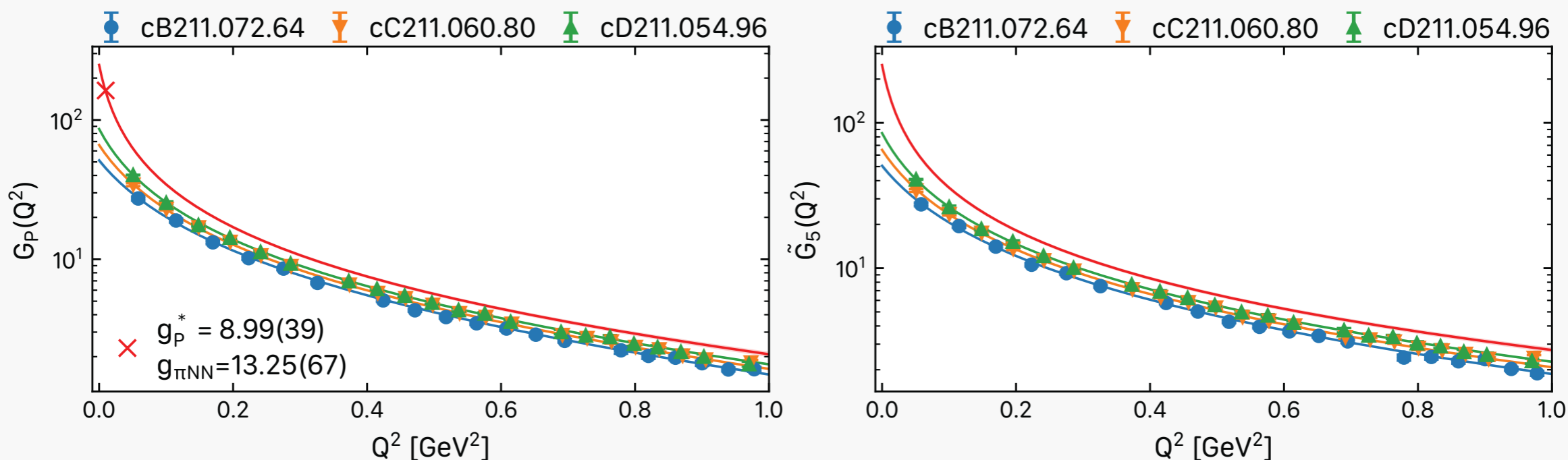
ETM collab., Phys. Rev. D 109 (2024) 3, 034503 [[arXiv:2309.05774](https://arxiv.org/abs/2309.05774)]

# Axial & Pseudoscalar form factors

Matrix element:

$$\langle N(p', s') | \bar{u} \gamma_5 u - \bar{d} \gamma_5 d | N(p, s) \rangle = \bar{u}(p', s') \gamma_5 G_5(Q^2) u(p, s)$$

Pseudoscalar form factor ( $G_5$ )



$$g_{\pi NN} = G_{\pi NN}(-m_\pi^2), \quad g_P^* = \frac{m_\mu}{2m_N} G_P(0.88m_\mu^2) \quad \tilde{G}_5(Q^2) = \frac{4m_N}{m_\pi^2} m_q G_5(Q^2)$$

$$\frac{F_\pi m_\pi^2}{m_\pi^2 + Q^2} G_{\pi NN}(Q^2) = m_q G_5(Q^2)$$

# Axial & Pseudoscalar form factors

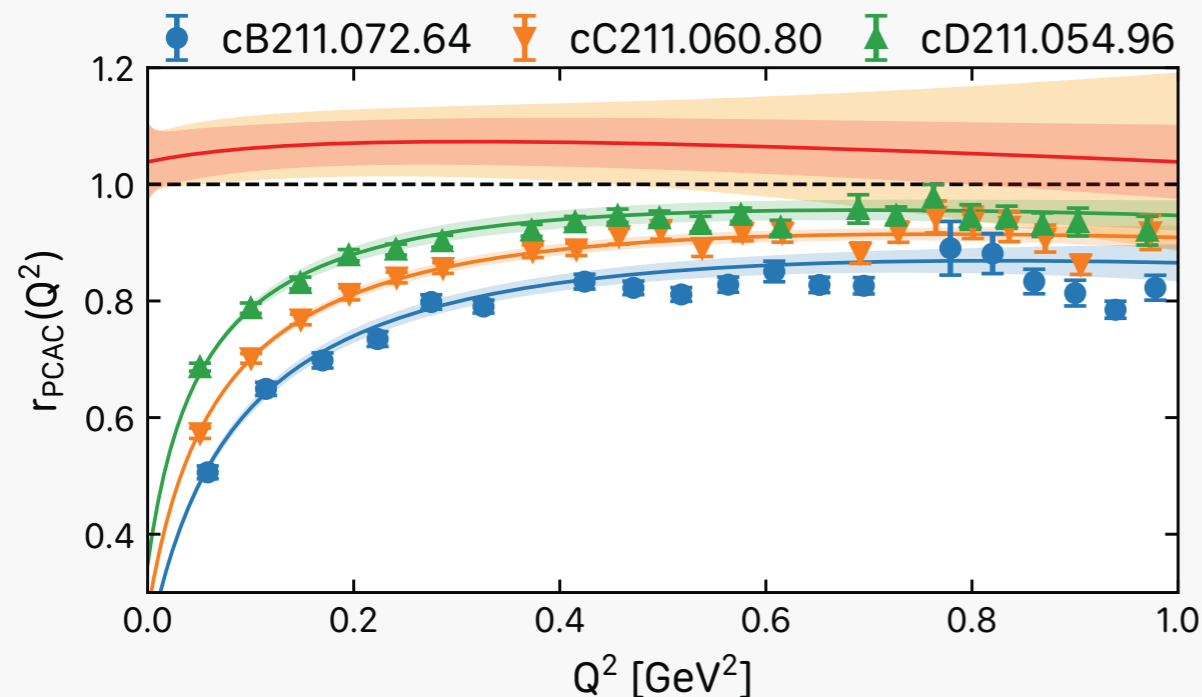
Check relation between axial and pseudoscalar form factors

- From PCAC relation

$$\partial^\mu A_\mu = 2m_q P$$

- Between nucleon states:

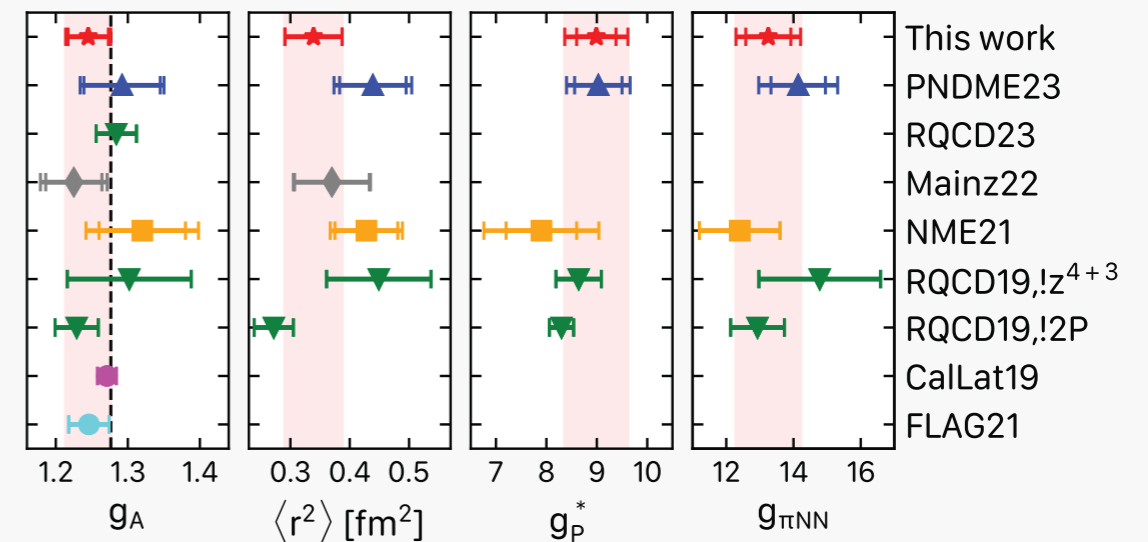
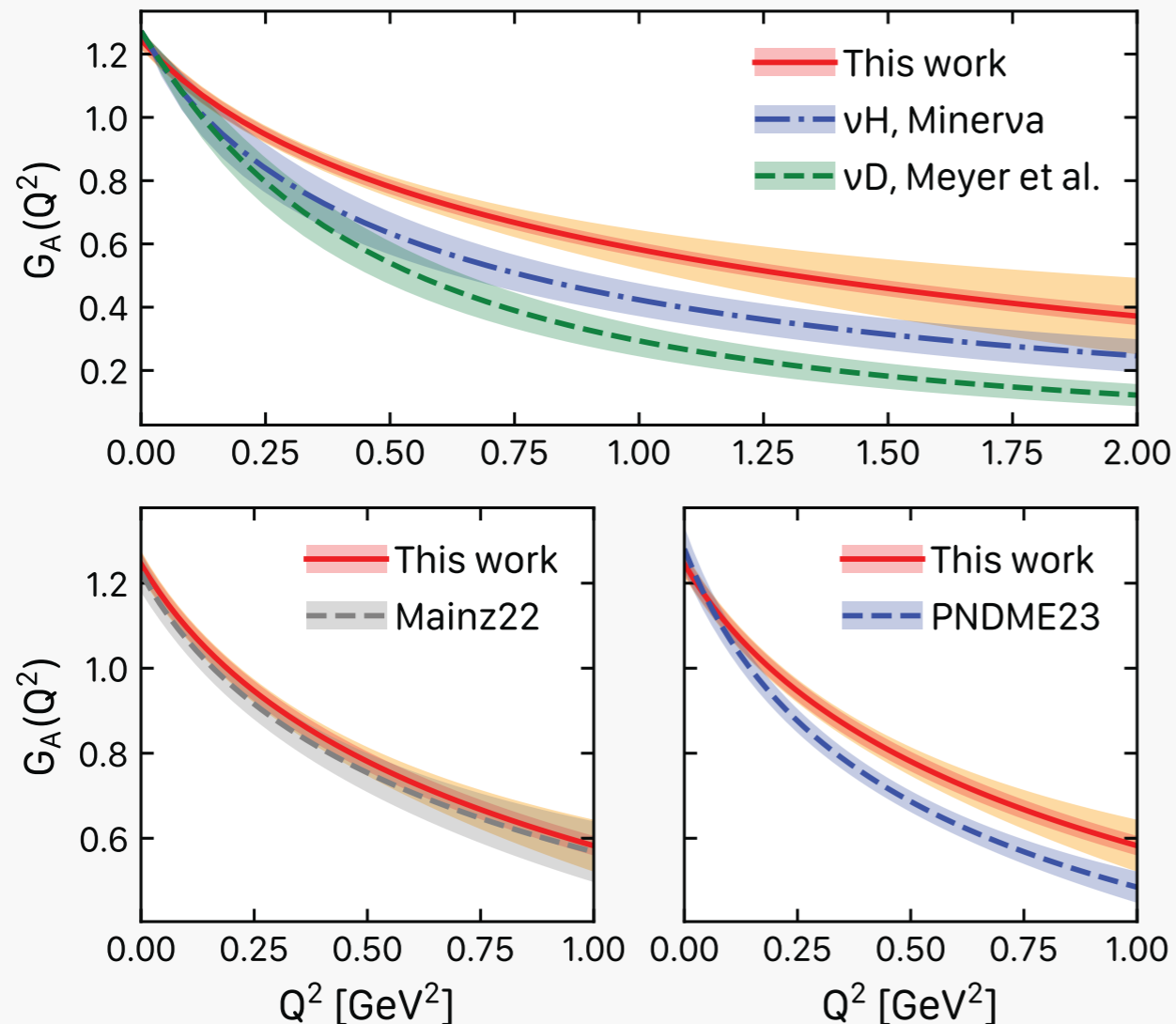
$$G_A(Q^2) - \frac{Q^2}{4m_N^2} G_P(Q^2) = \frac{m_q}{m_N} G_5(Q^2)$$



- Relation from PCAC restored at continuum limit ( $a \rightarrow 0$ )

# Axial & Pseudoscalar form factors

Comparison with experiment and other lattice results



- Good agreement between lattice results (*non-trivial*: each has varying systematics)
- Note the MINER $\nu$ A result (2023):
  - $r_A = 0.73(17)$  fm or
  - $(r_A)^2 = 0.53(25)$  fm<sup>2</sup>

# Summary & Outlook

- Lattice QCD with physical point ensembles at multiple lattice spacings
  - Here, three lattice spacings → Continuum limit directly at physical point
- Reproduction of well-known nucleon structure quantities, e.g. axial charge
- Requires thorough study of systematic uncertainties
  - Main systematic is excited state effects
- Reproduction of quantities known well experimentally at physical point
  - Axial charge and proton electromagnetic form factors
- Impact on quantities less well-known
  - $\sigma$ -terms, tensor charge, axial form factors, strange and charm contents

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