

Hadron structure from lattice QCD



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STIMULATE
European Joint Doctorates

Probing baryon weak decays
Warsaw, 6 March 2023

Outline

✳ Introduction

- **State-of-the-art lattice QCD simulations**

✳ 3D structure of the nucleon

- ➡ **Electromagnetic form factors and strangeness of the nucleon**
- ➡ **Axial form factors**
- ➡ **Direct computation of parton distributions (talk by K. Cichy)**

✳ Conclusions

Quantum Chromodynamics (QCD)

✳️ QCD-Gauge theory of the strong interaction

✳️ Lagrangian: formulated in terms of quarks and gluons

$$\mathcal{L}_{QCD} = -\frac{1}{4} F_{\mu\nu}^a F^{a\mu\nu} + \sum_{f=u,d,s,c,b,t} \bar{\psi}_f (i\gamma^\mu D_\mu - m_f) \psi_f \quad D_\mu = \partial_\mu - ig \frac{\lambda^a}{2} A_\mu^a$$



Harald Fritzsch



Murray Gell-Mann

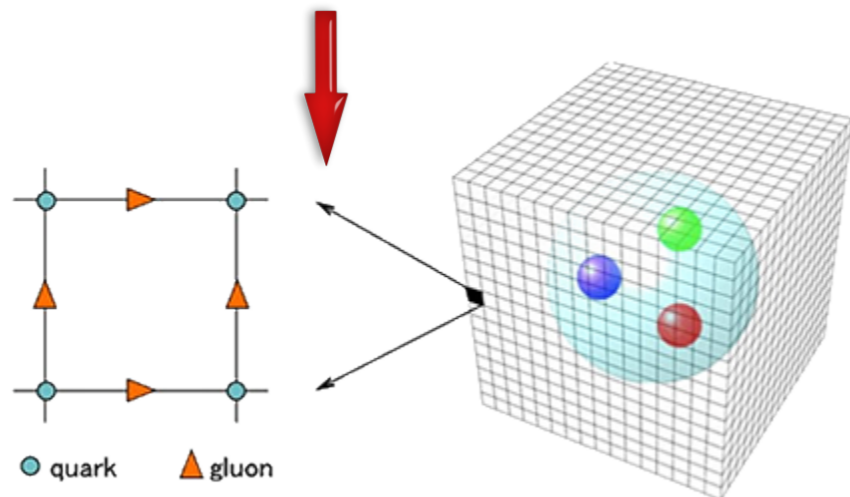


Heinrich Leutwyler

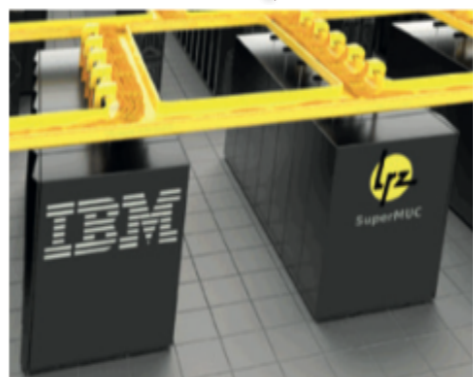
Phys. Lett. 47B (1973) 365

Lattice QCD

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



Simulation of gauge ensembles $\{U\}$

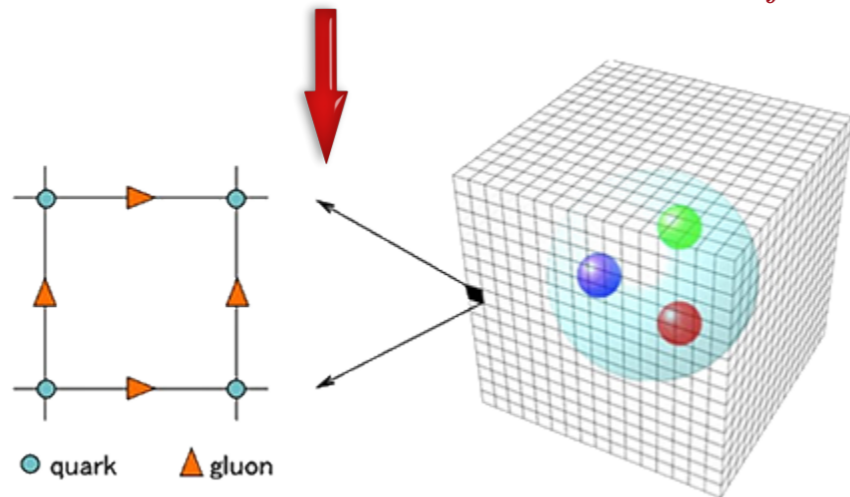


Quark & gluon propagators

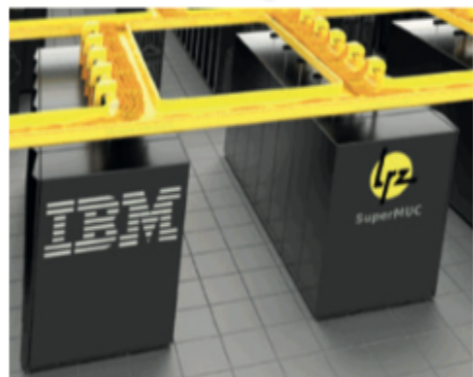


Lattice QCD

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



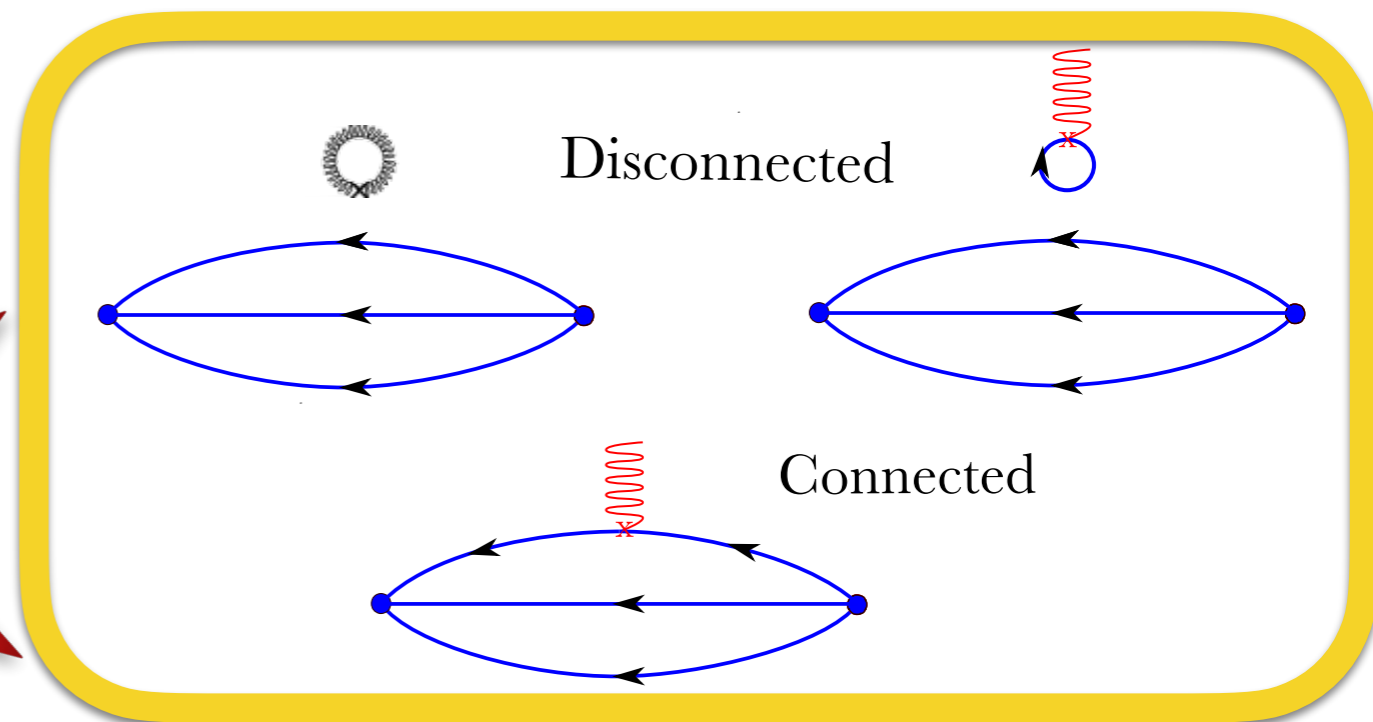
Simulation of gauge ensembles $\{U\}$



Quark & gluon propagators

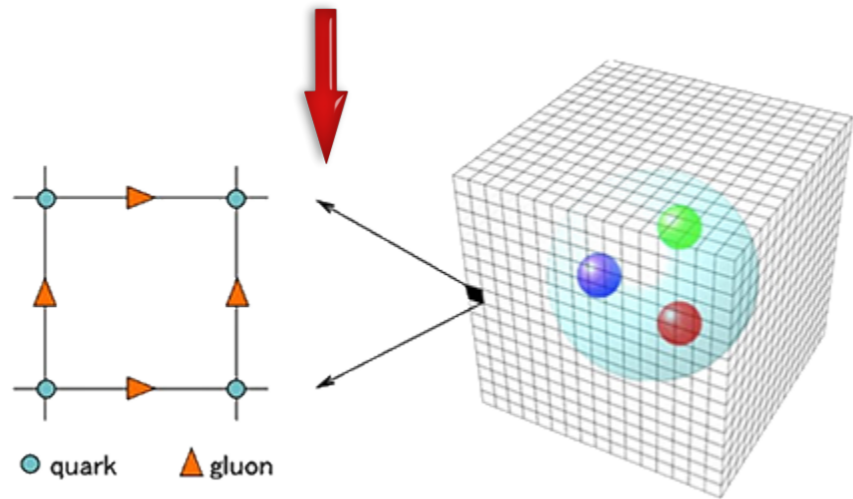


contractions

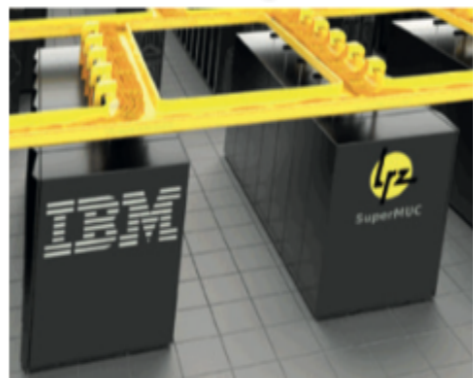


Lattice QCD

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



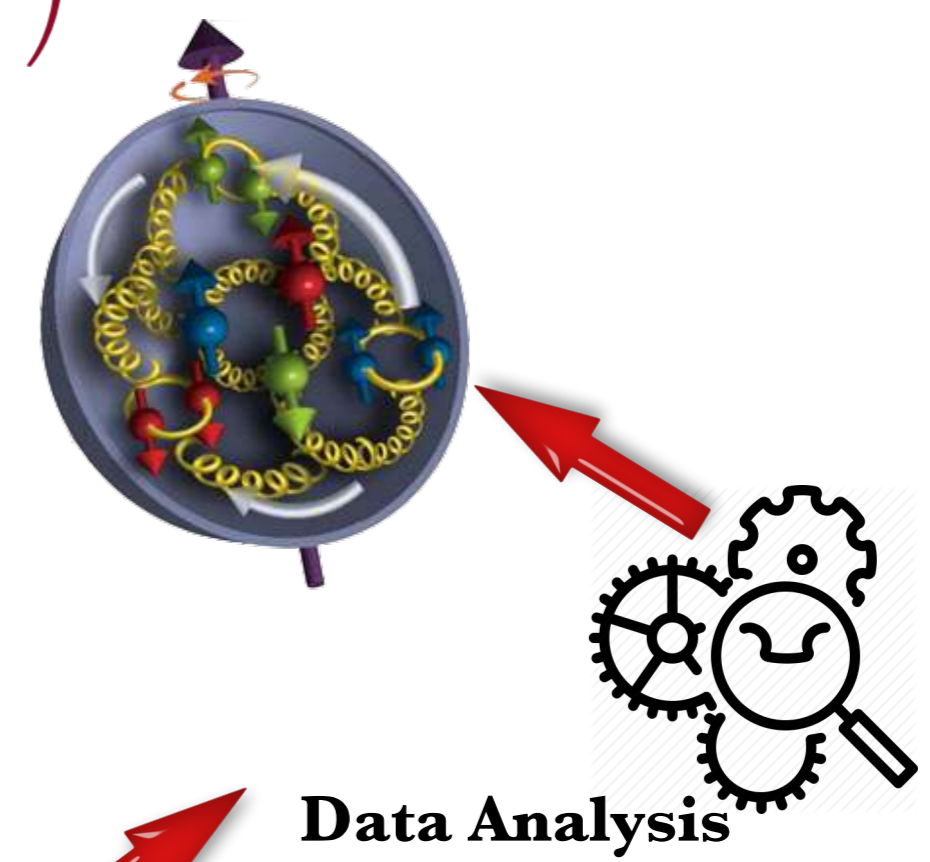
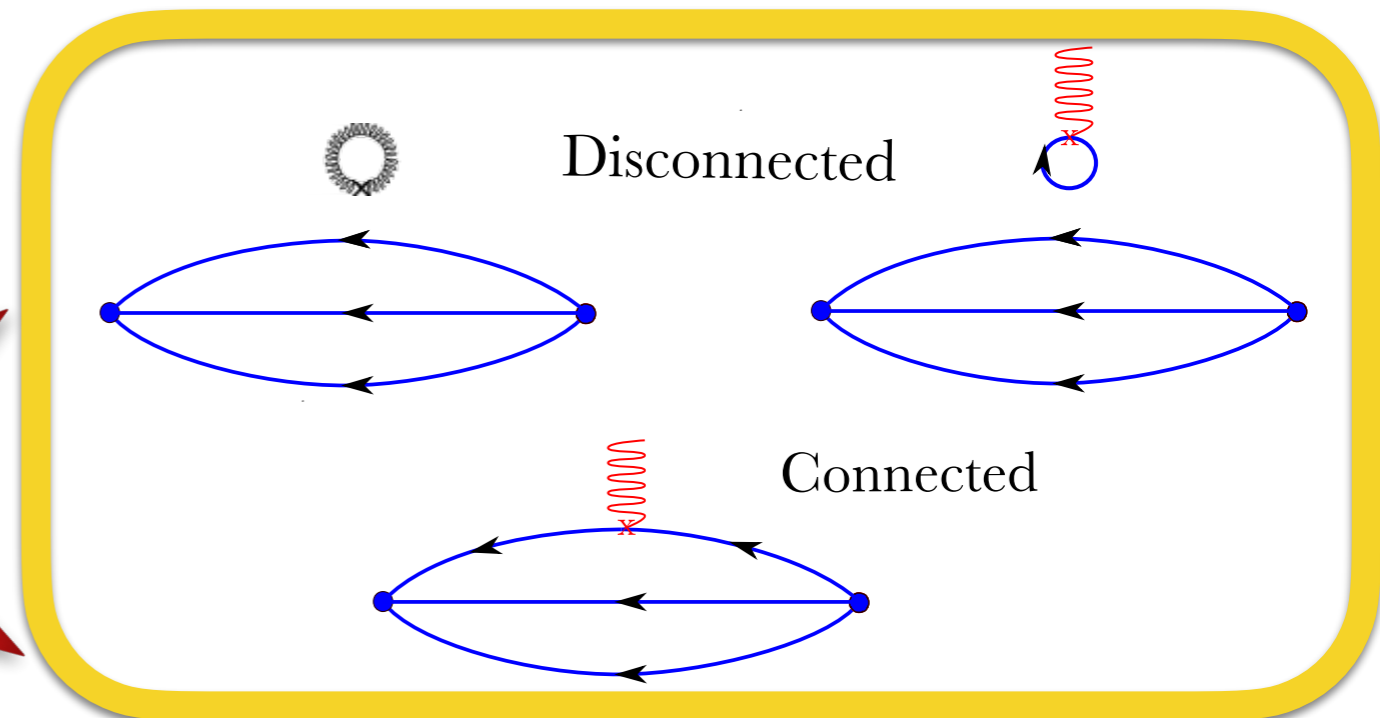
Simulation of gauge ensembles $\{U\}$



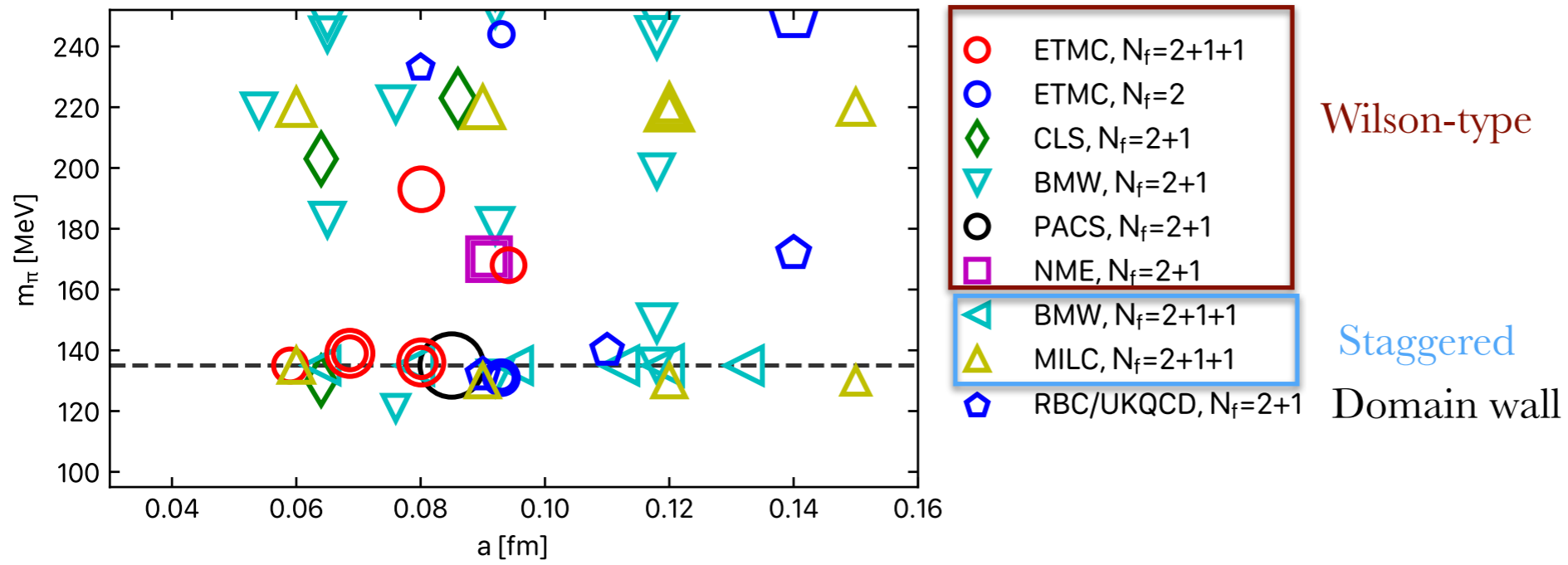
Quark & gluon propagators



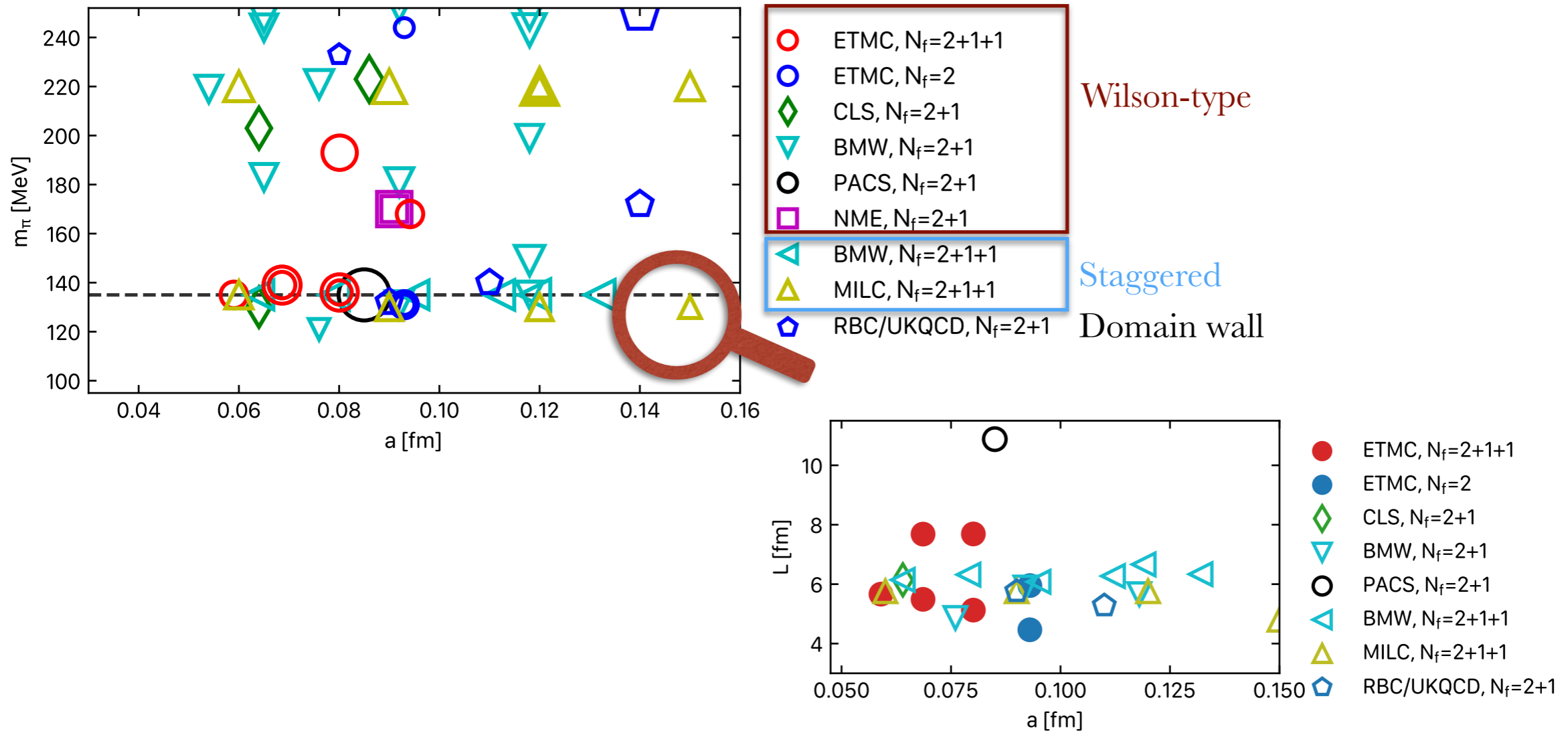
contractions



Status of current simulations



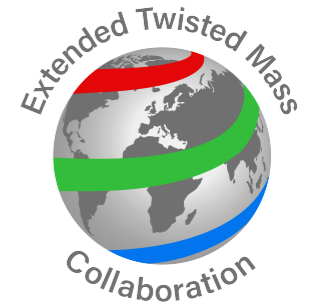
Status of current simulations



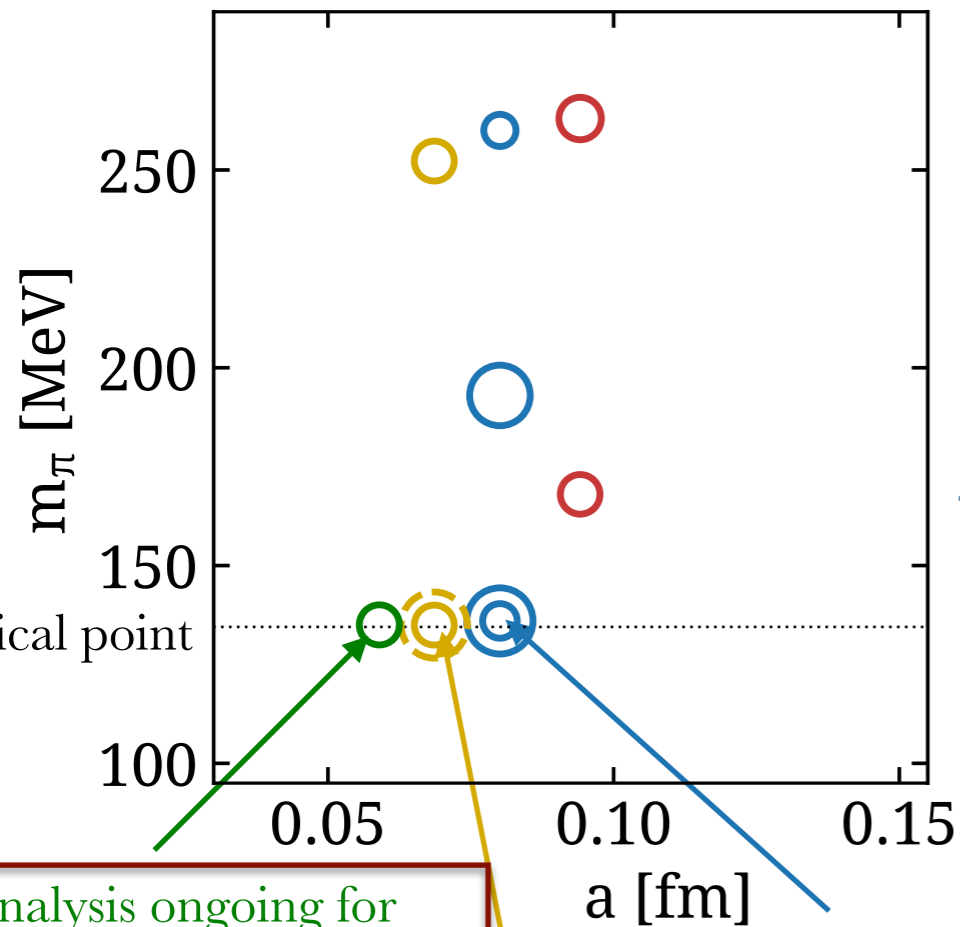
- ✿ A number of collaborations has generated gauge ensembles with physical values of the u/d, s and c quarks
- ✿ Algorithmic improvements needed to simulate for $a < 0.05$ fm due to critical slow down in Markov chain Monte Carlo (long autocorrelations) —> new sampling algorithms, e.g. flow-based algorithms

G. Kanwar *et al.*, Phys. Rev. Lett. 125 (2020) 121601, arXiv:2003.06413; D. Boyda *et al.*, Phys.Rev.D 103 (2021) 074504, arXiv:2008.05456; M. S. Albergo *et al.*, Phys.Rev.D 104 (2021) 114507, arXiv:2106.05934, J. Finkenrath arXiv:2201.02216

Gauge ensembles generated by ETMC



$N_f=2+1+1$ ETMC ensembles



✱ 5 ensembles at physical pion mass

- 3 lattice spacings $0.05 < a < 0.1$ fm \rightarrow take continuum limit **directly at the physical point** avoiding chiral extrapolation removing a major systematic error in the baryon sector
- Two volumes at $a=0.08$ fm and 0.07 fm of $L_{m_\pi} \sim 3.6$ (5.1 fm) and $L_{m_\pi} \sim 5.4$ (7.7 fm)

✱ Algorithmic improvements needed to go to $a < 0.05$ fm due to critical slow down in HMC (long autocorrelations) \rightarrow new approaches e.g. Machine learning approaches using equivariant flows

G. Kanwar, et al., Phys. Rev. Lett. 125 (2020) 121601, arXiv:2003.06413; D. Boyda, et al., Phys.Rev.D 103 (2021) 074504, arXiv: 2008.05456; M. S. Albergo *et al.*, Phys.Rev.D 104 (2021) 114507, arXiv:2106.05934

Analysis ongoing for $96^3 \times 192$, $a \sim 0.06$ fm -D96

• Analysis completed for $64^3 \times 128$ $a=0.08$ fm -B64

• Analysis ongoing for $96^3 \times 192$ $a=0.08$ fm

• Analysis ongoing for $80^3 \times 160$, $a=0.07$ fm -C80

• Simulation ongoing for $112^3 \times 224$, $a=0.07$ fm

Systematics & Challenges

- * **Simulations directly at the physical point** ✓



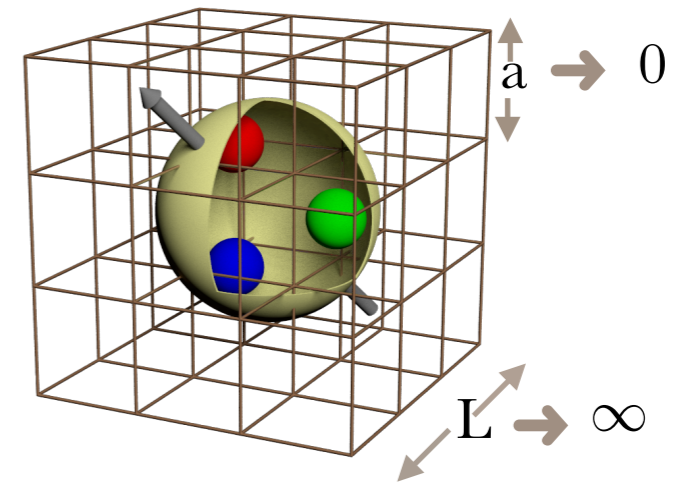
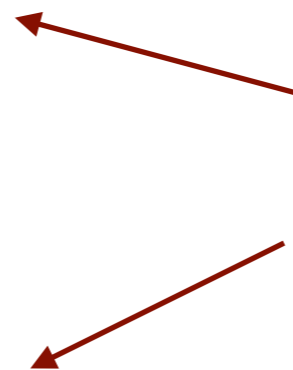
Systematic effects from chiral extrapolation are eliminated

- * **Discretisation effects:** Continuum limit

—> need simulations for at least 3 lattice spacings

- * **Finite volume effects:** Infinite volume limit

—> need simulations for at least 3 volumes



- * **Renormalisation** ✓



Non-perturbatively with improvements e.g using perturbative subtraction of lattice artefacts

- * **Ground-state identification**

Cross-check (one-, two- and three-state fits, summation)

Two-particle state contribution complicate the identification of the ground state

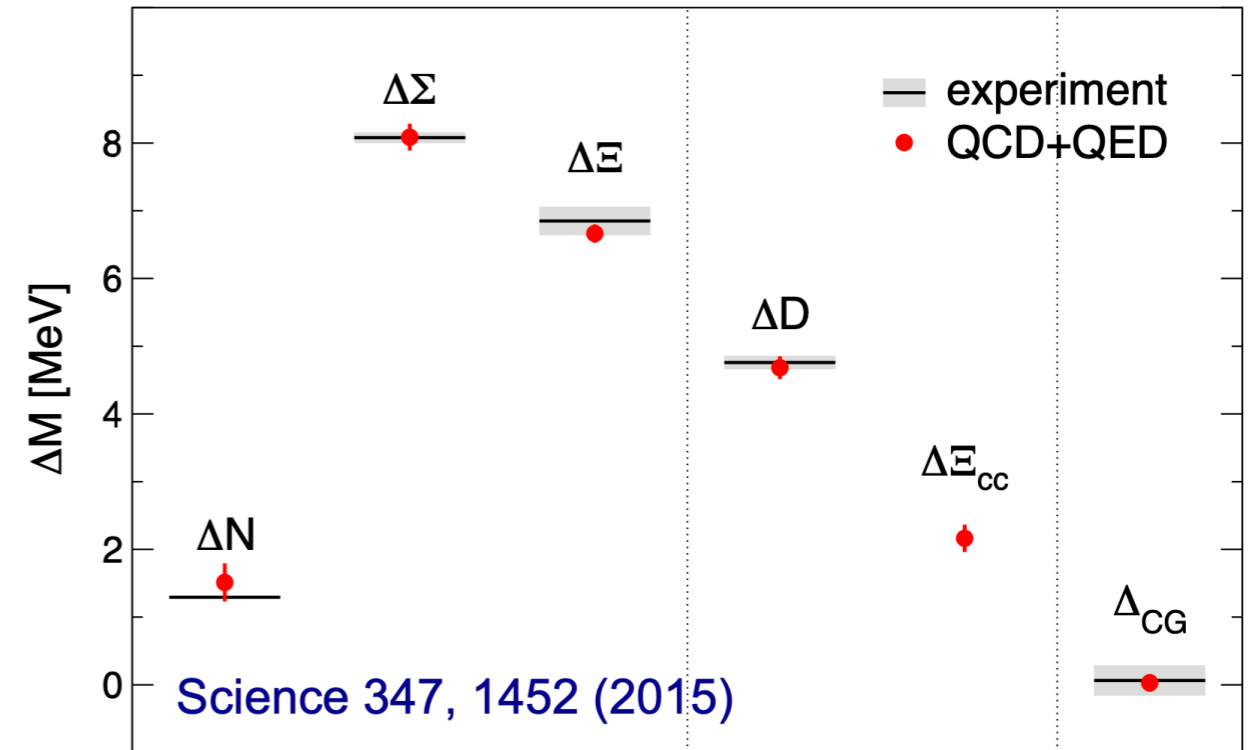
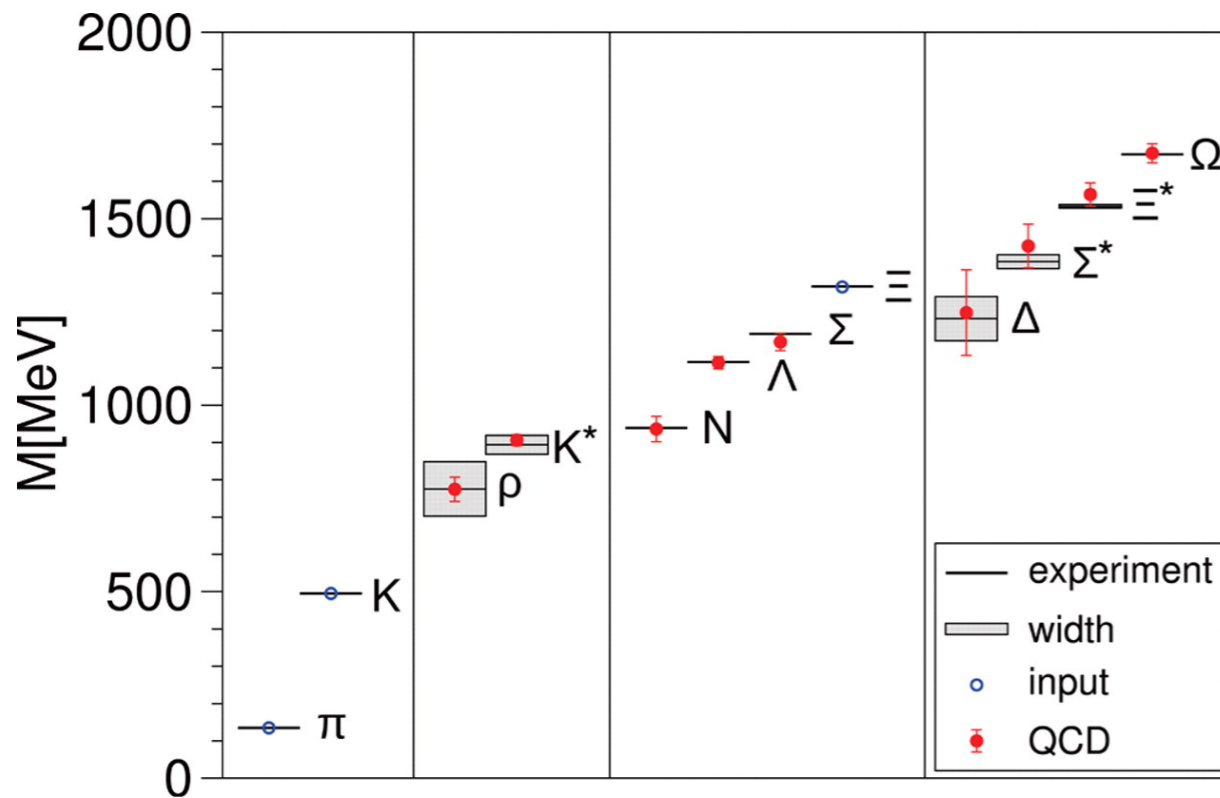
- * In what follows we assume **isospin symmetry** i.e. up and down quarks have equal mass, and **neglect EM effects**

Low-lying hadron spectrum

✳ BMW collaboration determined the low-lying hadron masses, as well as the mass splittings

S. Durr *et al.*, Science 322 (2008) 1224

Sz. Borsanyi *et al.*, Science 347 (2015) 1452



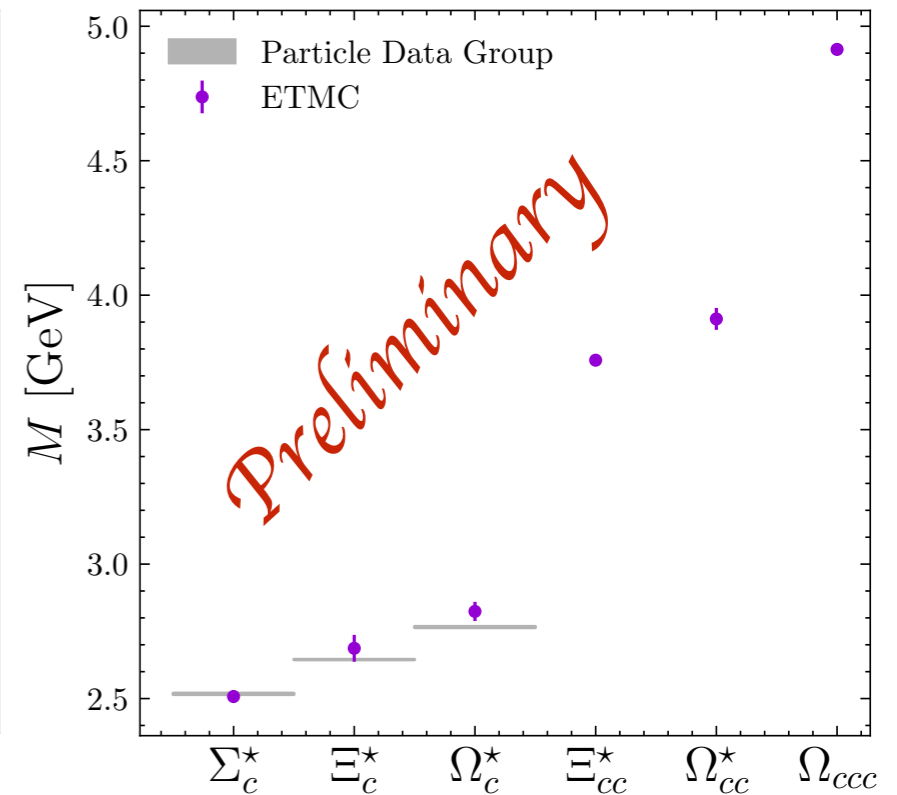
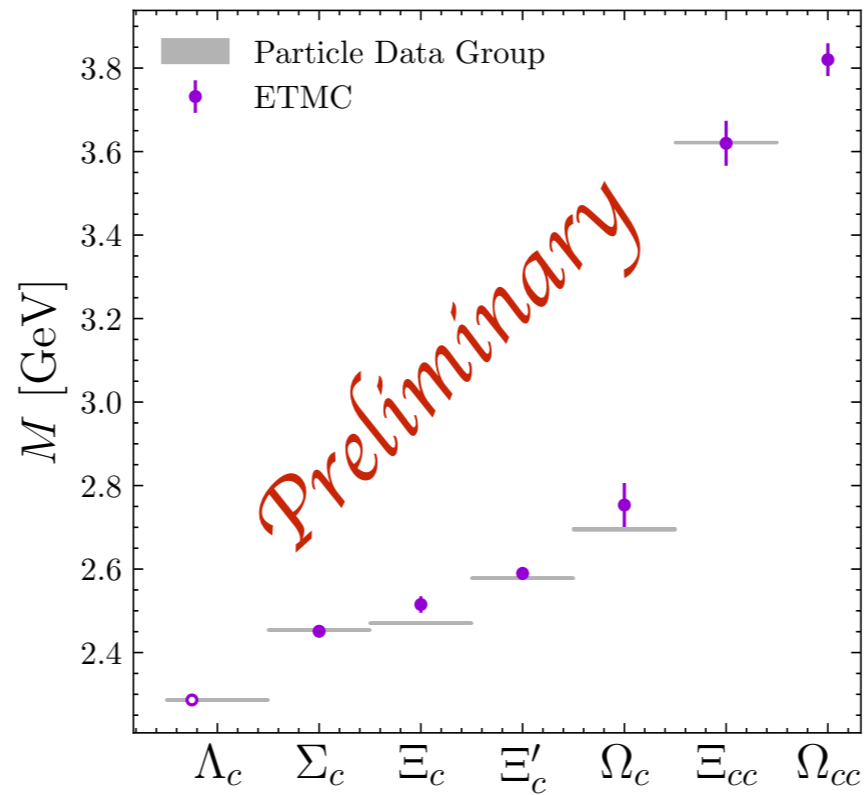
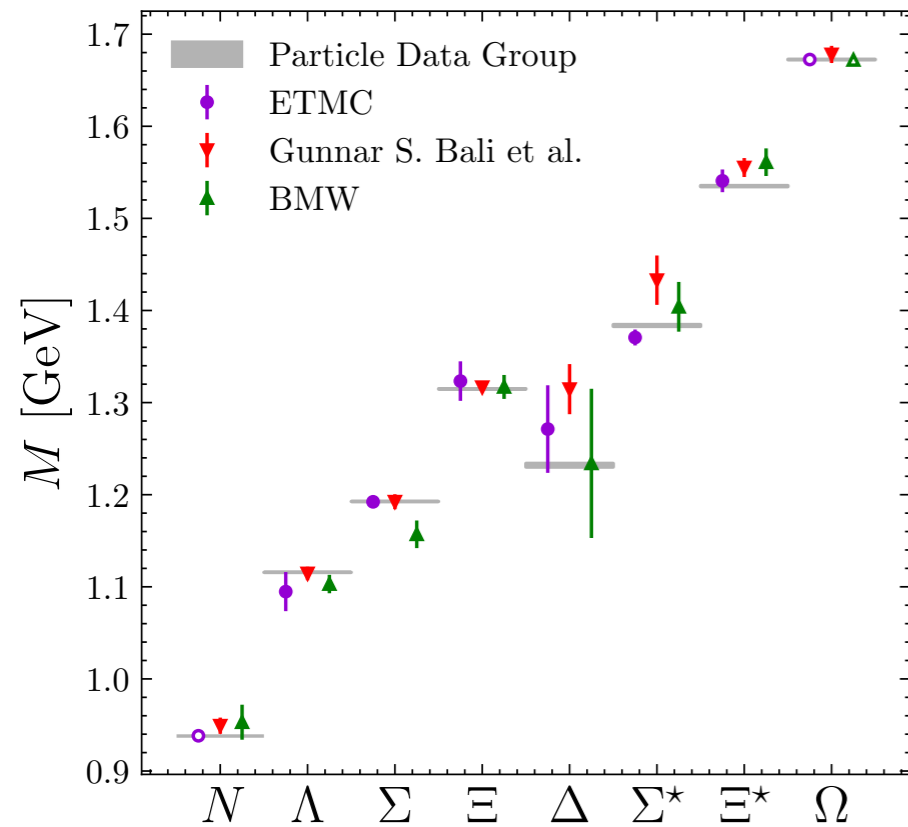
	mass splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta \Sigma = \Sigma^- - \Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta \Xi = \Xi^- - \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^\pm - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta \Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^+$	2.16(11)(17)	-2.53(11)(06)	4.69(10)(17)
$\Delta_{CG} = \Delta N - \Delta \Sigma + \Delta \Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

Lattice QCD reproduces the low-lying hadron masses and mass splittings

Recent results on the low-lying masses

✳ ETMC: only using physical point ensembles \rightarrow no uncontrolled systematics due to chiral extrapolation


✳ RQCD: extrapolated to the physical pion mass



Baryonic semi-leptonic decays

Write transition matrix elements $H \rightarrow H' l \bar{\nu}_l$ in term of hadronic J^h and leptonic J^l components

$$\mathcal{M}_{H \rightarrow H' l \bar{\nu}} = \frac{G_F}{\sqrt{2}} C \langle H' | J_\mu^h | H \rangle \langle l | J^{\mu, l} | \bar{\nu}_l \rangle$$


 Relevant Cabibbo angle

V-A structure and for u, d and s quarks and each current we have $\Delta S=0$ and $\Delta S=1$ components

$$\langle H' | J_\mu^h | H \rangle = \langle H' | V_\mu - A_\mu | H \rangle$$

The matrix elements in Euclidean space are written as

$$\langle H'(\vec{p}', s') | V_\mu | H(\vec{p}, s) \rangle = \bar{u}_{H'}(\vec{p}', s') \left[\gamma_\mu f_1(q^2) + i\sigma_{\mu\nu} q_\nu \frac{f_2(q^2)}{M_H + M_{H'}} - q_\mu \frac{f_3(q^2)}{M_H + M_{H'}} \right] u_H(\vec{p}, s)$$

$$\langle H'(\vec{p}', s') | A_\mu | H(\vec{p}, s) \rangle = \bar{u}_{H'}(\vec{p}', s') \left[\gamma_\mu \gamma_5 g_1(q^2) + i\sigma_{\mu\nu} q_\nu \gamma_5 \frac{g_2(q^2)}{M_H + M_{H'}} - q_\mu \gamma_5 \frac{g_3(q^2)}{M_H + M_{H'}} \right] u_H(\vec{p}, s)$$

- At $q^2=0$ we get the vector and axial coupling constants: $f_1(0) = g_V$ $g_1(0) = g_A$
- For diagonal matrix elements the form factors $f_3(q^2)$ and $g_3(q^2)$ vanish as they do in the SU(3) limit

$$n \rightarrow pe^- \bar{\nu}; \quad \Sigma^- \rightarrow ne^- \bar{\nu}; \quad \Xi^- \rightarrow \Lambda e^- \bar{\nu}; \quad \Lambda \rightarrow pe^- \bar{\nu}; \quad \dots$$

Most studied in lattice QCD

Very few lattice studies on the rest

$$\Xi^0 \rightarrow \Sigma^+ e^- \bar{\nu}; \quad \Sigma^- \rightarrow ne^- \bar{\nu}$$

S. Sasaki, 1209.6115;

M. Goeckeler *et al.* (QCDSF) 1101.2806;

A. N. Cooke *et al.*, 1311.4916 and 1212.2564; P.E. Shanahan *et al.*, 1508.06923.

Nucleon matrix elements

$$\langle N(\vec{p}', s') | V_\mu | N(\vec{p}, s) \rangle = \bar{u}_N(\vec{p}', s') \left[\gamma_\mu F_1(q^2) + i \frac{\sigma_{\mu\nu} q_\nu}{2M_N} F_2(q^2) \right] u_N(\vec{p}, s)$$

Dirac Pauli

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

$$\langle N(\vec{p}', s') | A_\mu | N(\vec{p}, s) \rangle = \bar{u}_N(\vec{p}', s') \left[\gamma_\mu \gamma_5 G_A(q^2) - \frac{q_\mu \gamma_5}{2M_H} G_P(q^2) \right] u_N(\vec{p}, s)$$

Our work:

✳ Nucleon electromagnetic and axial form factors

✳ Δ transition form factors:

- Previous work not using state-of-the-art ensembles and Delta stable
- Formalism for unstable Delta developed, work is ongoing

✳ Delta electromagnetic and axial form factors - only done assuming stable Delta and older ensembles

Charges of baryons


- Readily accessible in lattice QCD
- Only recently we have results directly at the physical point (i.e. simulations with $m_\pi \sim 135 \pm 10$ MeV)

Nucleon isovector charges

$$g_V = \langle 1 \rangle_{u-d}$$

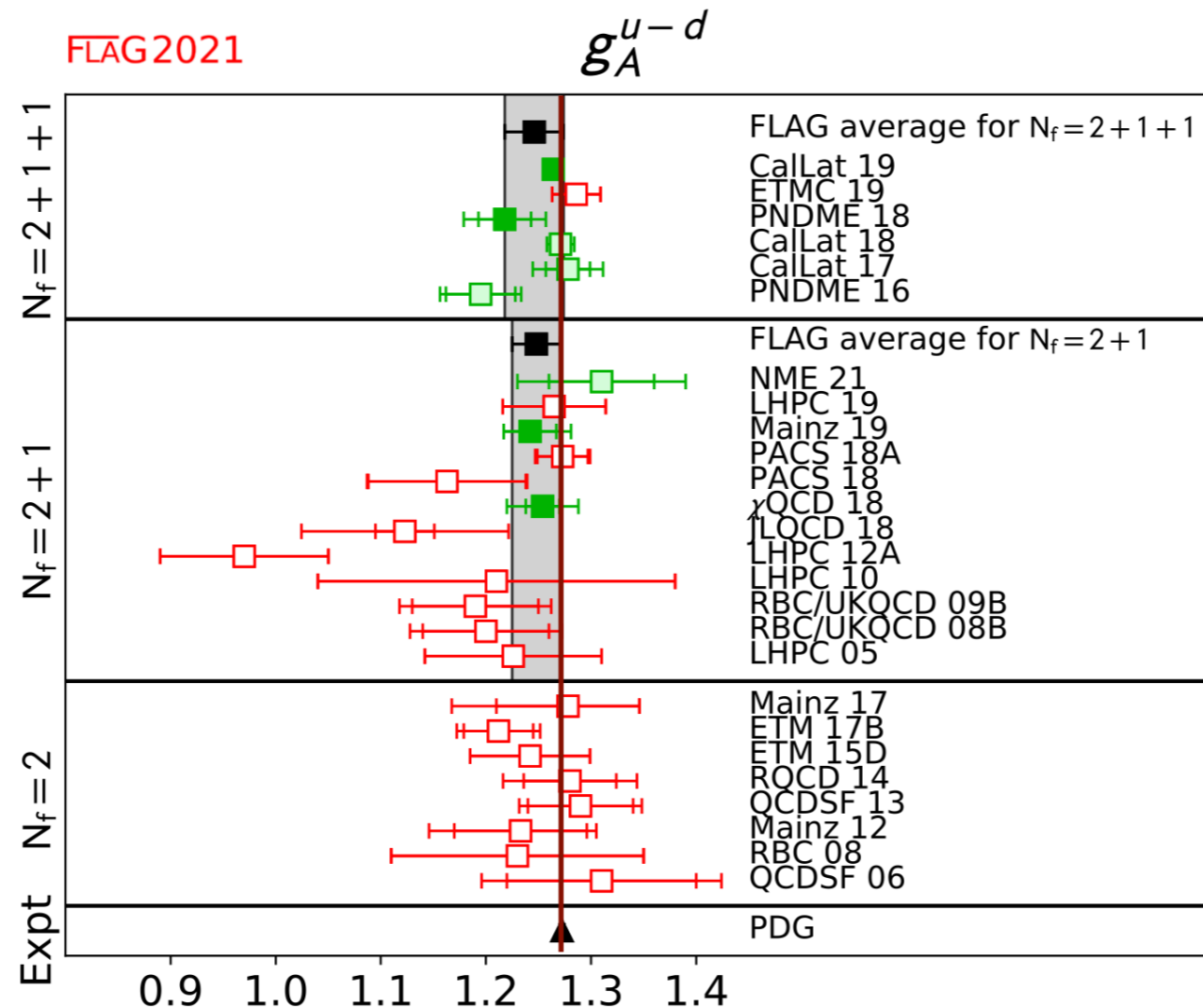
- $g_V = 1$

$$g_A = \langle 1 \rangle_{\Delta u - \Delta d}$$

- $g_A = 1.2723 \pm 0.0023$  reproduce

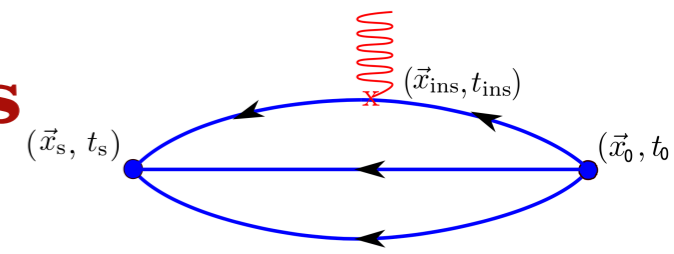
$$g_T = \langle 1 \rangle_{\delta u - \delta d}$$

- $g_T = 0.53 \pm 0.25$ M. Radici and A. Bacchetta. PRL 120 (2018) 192001



(1) Lattice QCD results on g_A consistent with experimental value

Nucleon isovector (u-d) axial and tensor charges

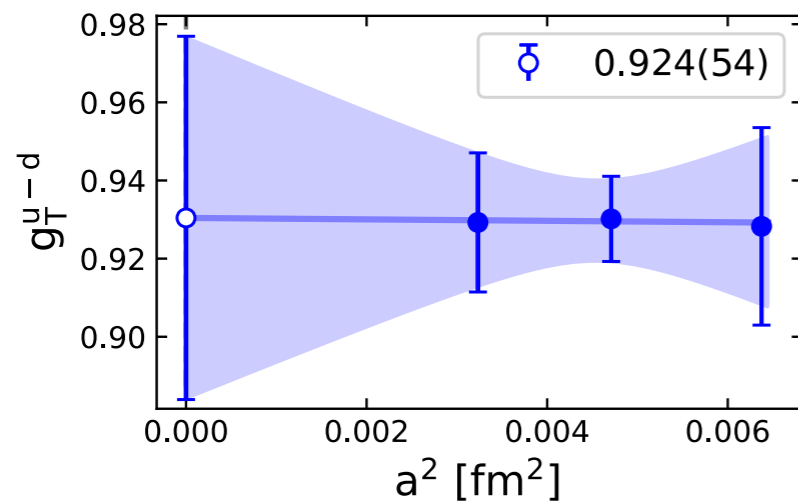
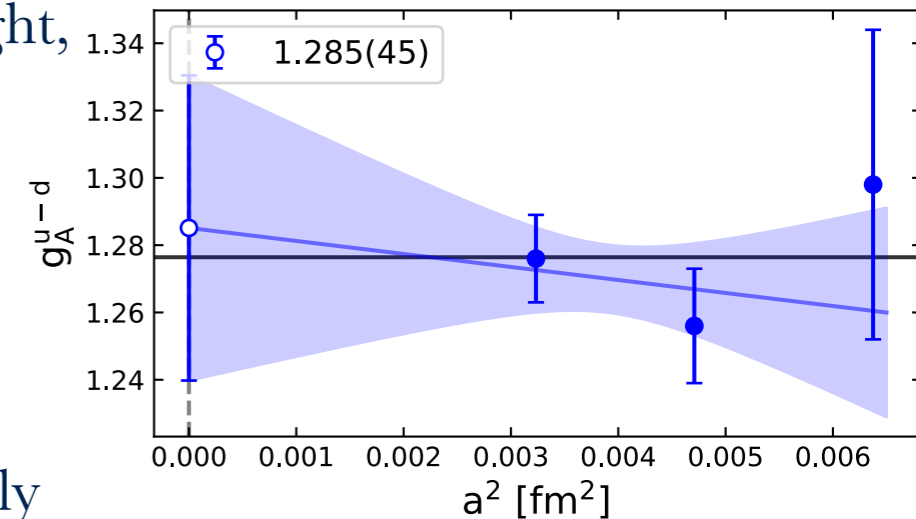


✳ Only connected contributions

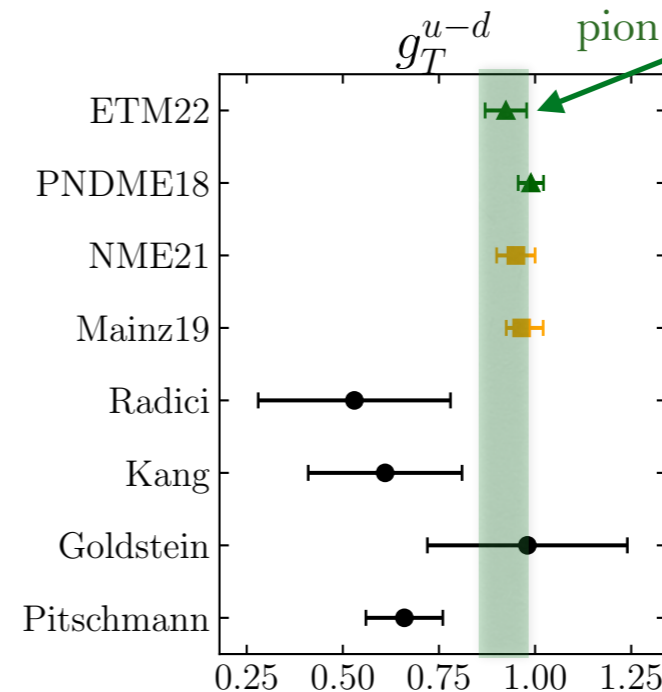
✳ Use three gauge ensembles generated using physical values of the light, strange and charm quarks:

- B64-ensemble: $64^3 \times 128$, $a \sim 0.08$ fm
- C80-ensemble: $80^3 \times 160$, $a \sim 0.07$ fm
- D96-ensemble: $96^3 \times 192$, $a \sim 0.06$ fm

✳ Obtain the tensor charge for the first time in the continuum using only physical point ensembles



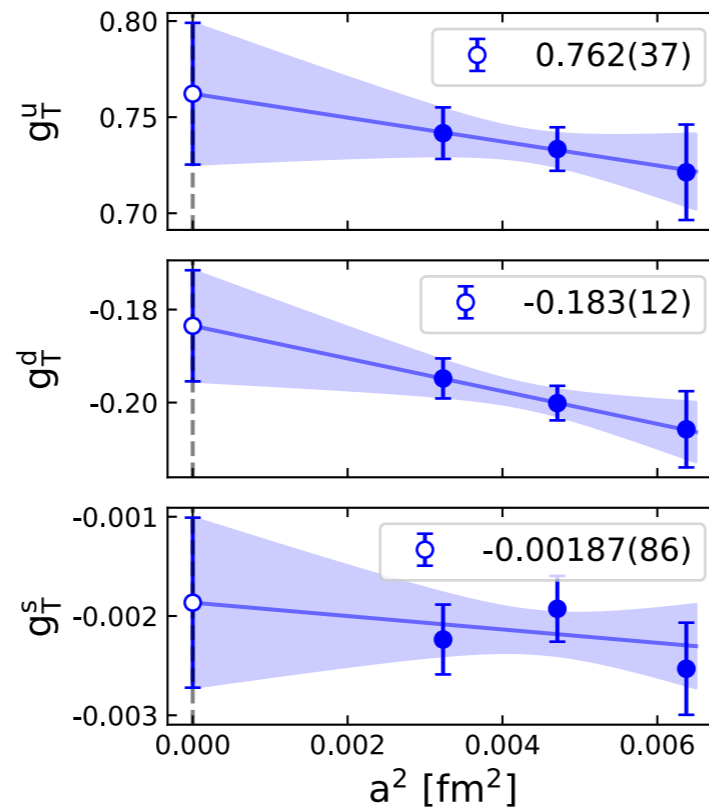
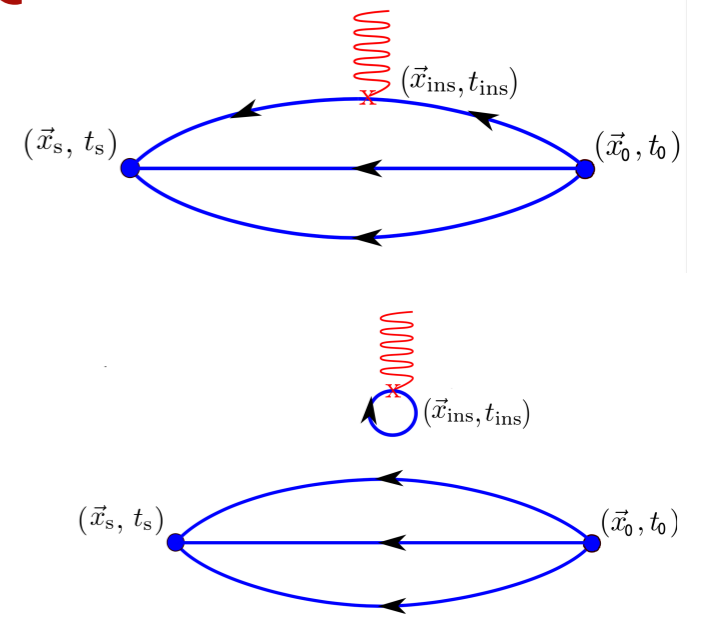
Continuum limit directly at physical pion mass



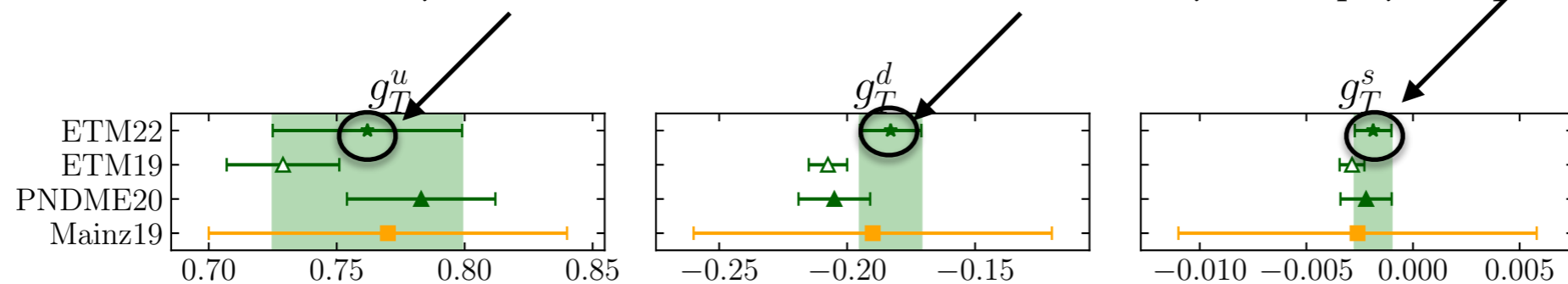
✳ Precision results on the isovector tensor charge - input for phenomenology e.g. JAM3D-22 analysis

Flavor diagonal tensor charge

- ✳ Evaluate both connected and disconnected contributions
- ✳ Obtain flavor diagonal tensor charge for the first time in the continuum using only physical point ensembles - input for phenomenology



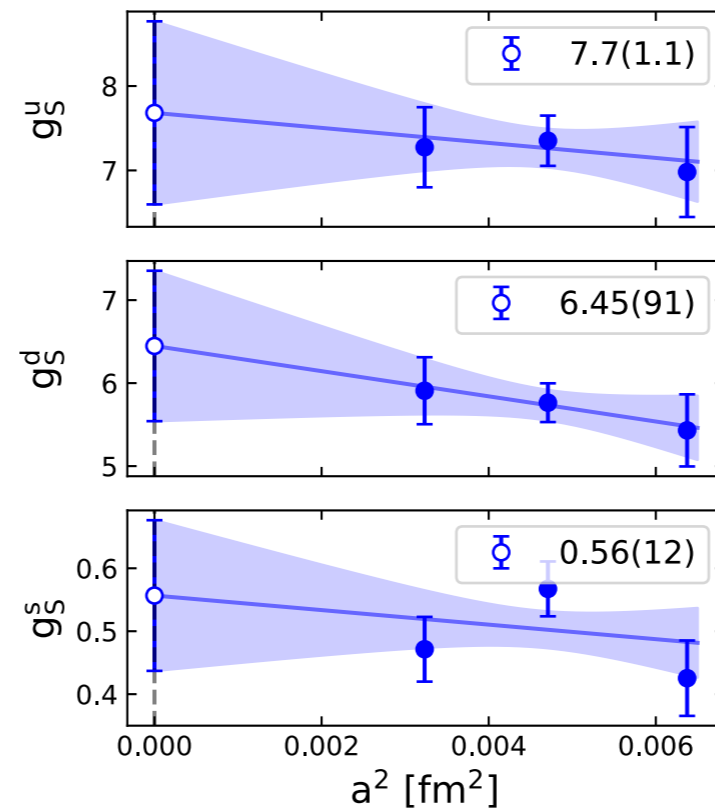
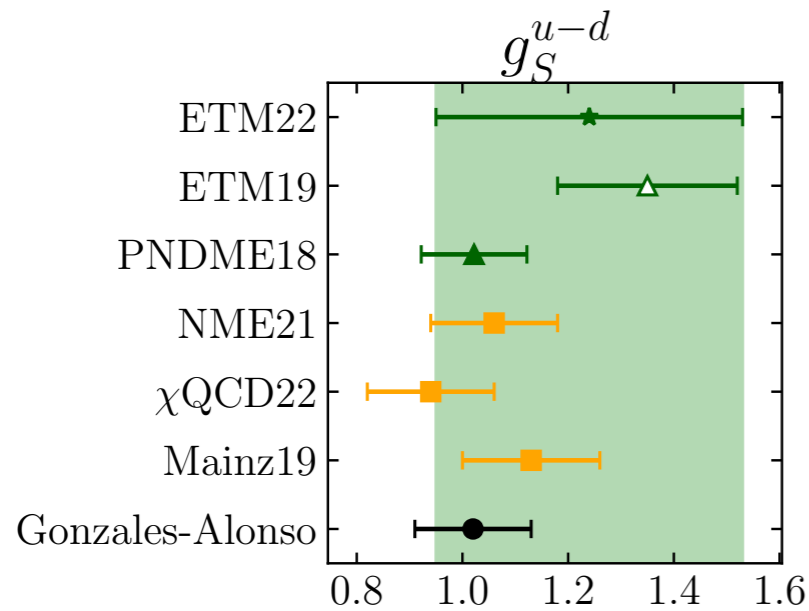
Only calculation in the continuum limit directly at the physical point



(2) Precision era of lattice QCD for charges including flavor diagonal

Nucleon scalar charge

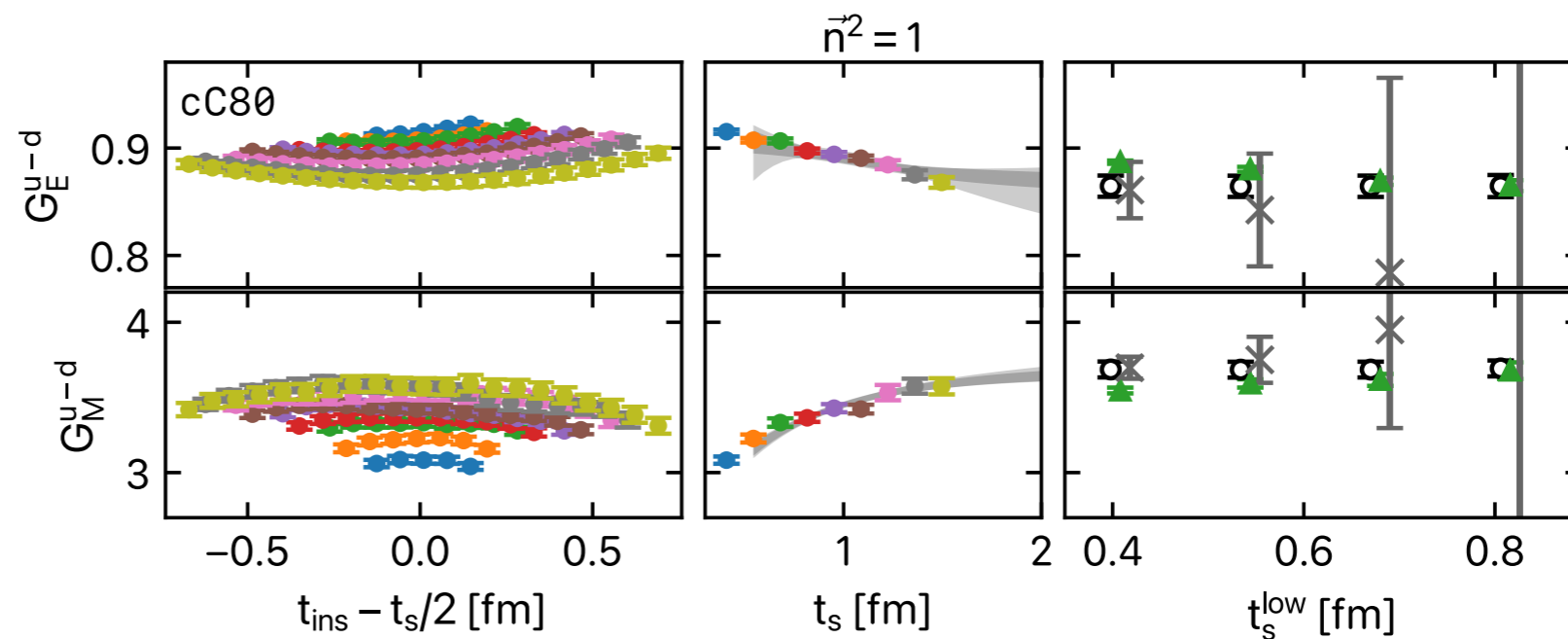
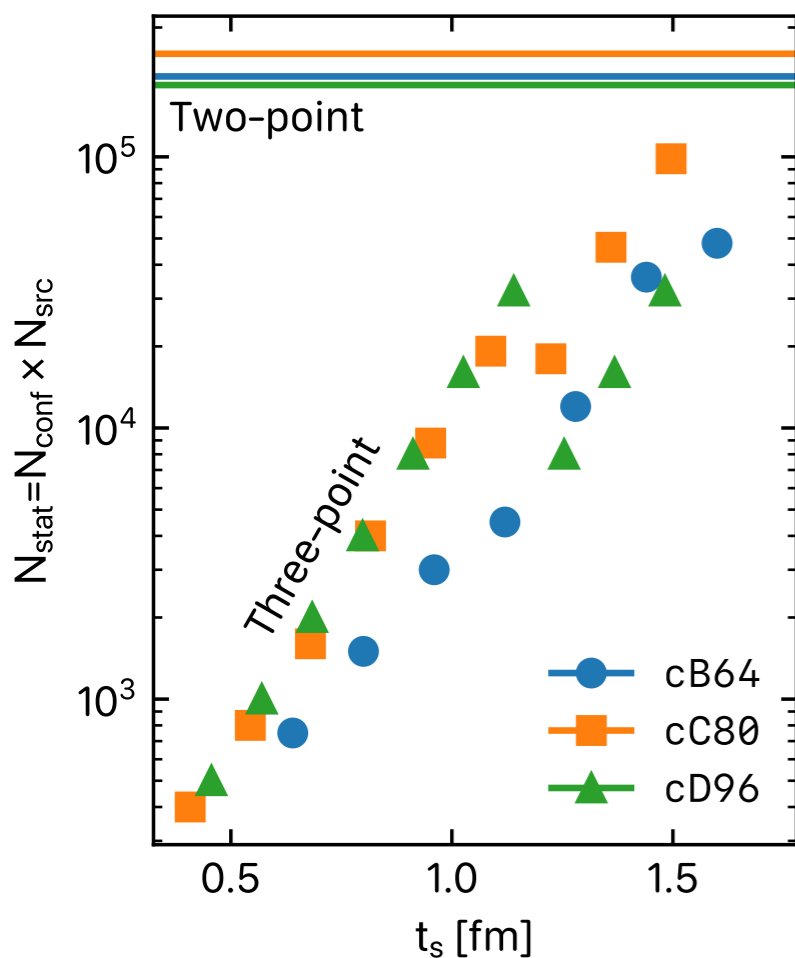
✳ Perform a similar analysis for the scalar charge - important input for direct dark matter searches



✳ Scalar charge is also directly related to the nucleon σ -terms or quark content $\sigma_q = m_q \langle N | \bar{q}q | N \rangle$

Electromagnetic form factors

- ★ Aim for *constant statistical errors* over all values of t_s of a given ensemble to enable excited state analysis
- ★ Large two-point functions needed for disconnected



▲ Summation

⊖ Two-state,
 $E_1(0) = \varepsilon_1(0)$
 $E_1(\vec{q}) = \varepsilon_1(\vec{q})$

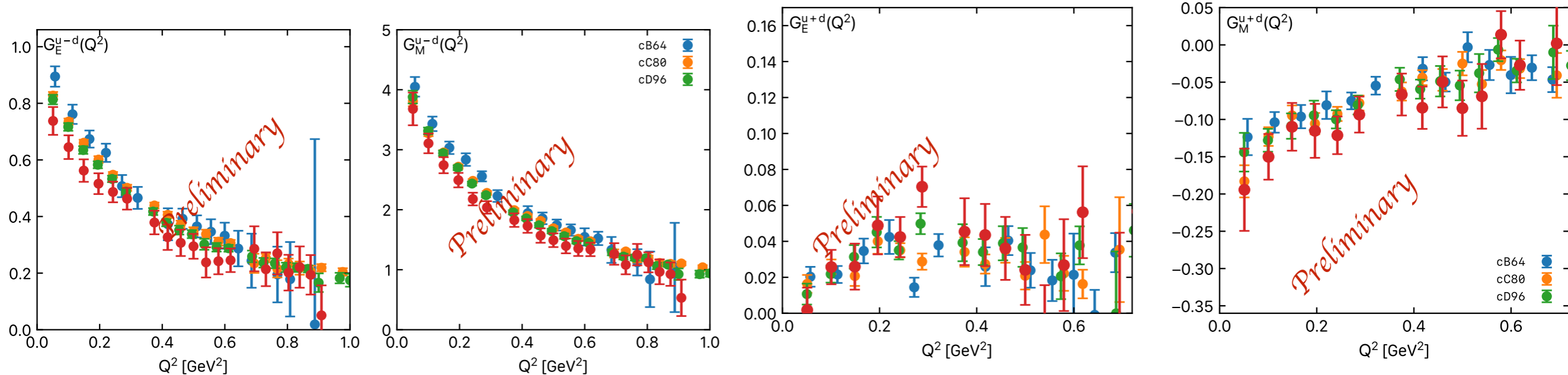
⊗ Two-state,
 $E_1(\vec{q}) \neq \varepsilon_1(\vec{q})$
 $E_1(0) \neq \varepsilon_1(0)$

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

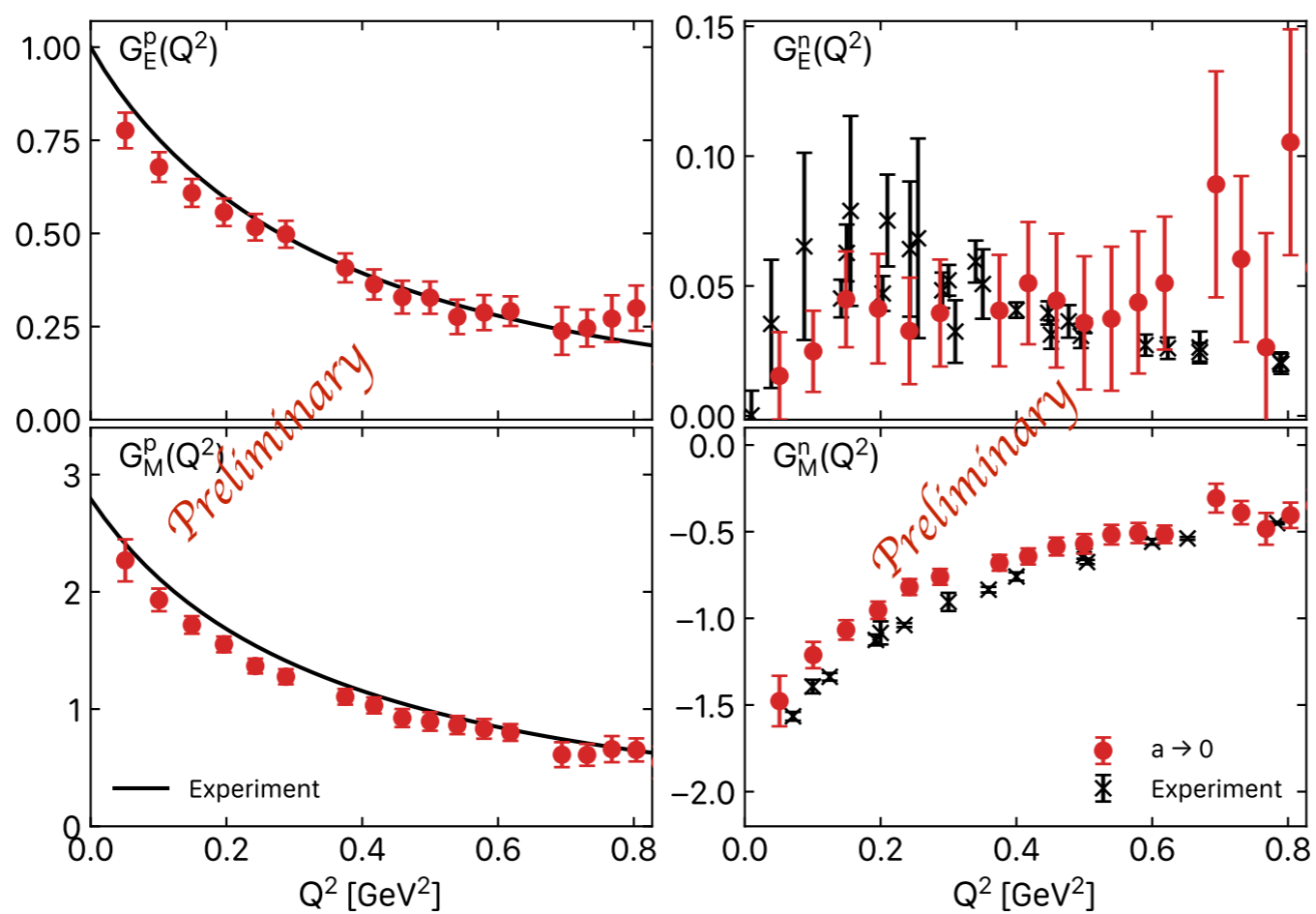
$$G(\vec{q}; t_s) = a_0(\vec{q}) e^{-\varepsilon_0(\vec{q})t_s} + a_1(\vec{q}) e^{-\varepsilon_1(\vec{q})t_s}$$

Continuum limit

Disconnected (u+d)



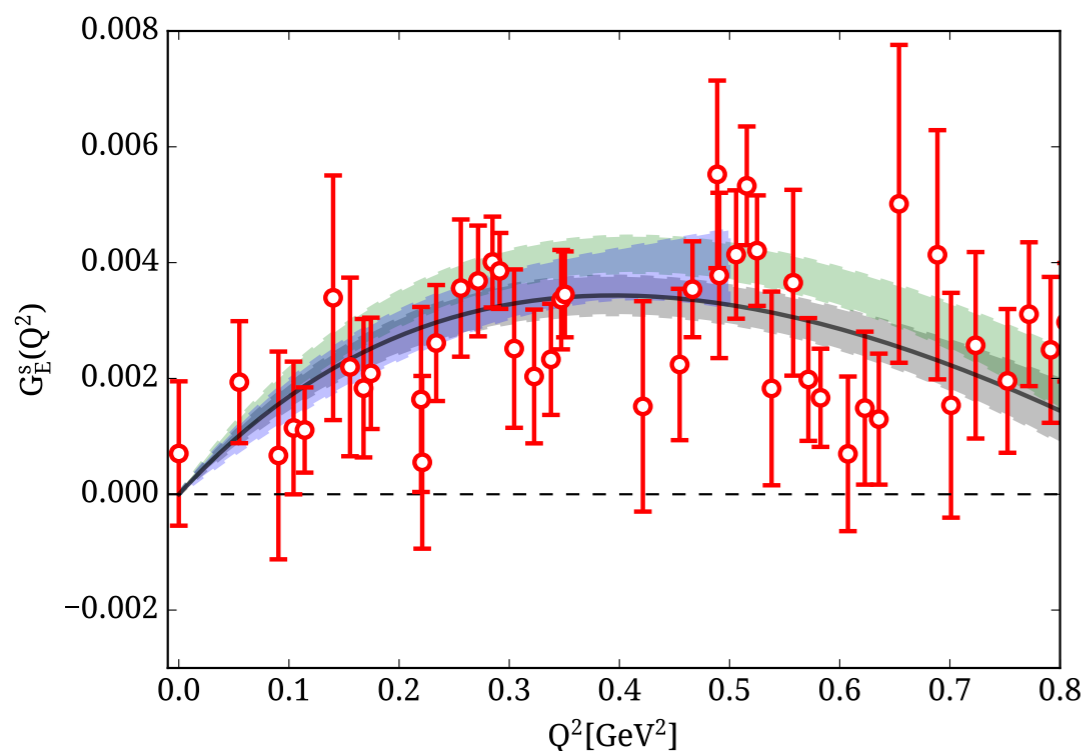
Proton and Neutron EM form factors compared to experiment



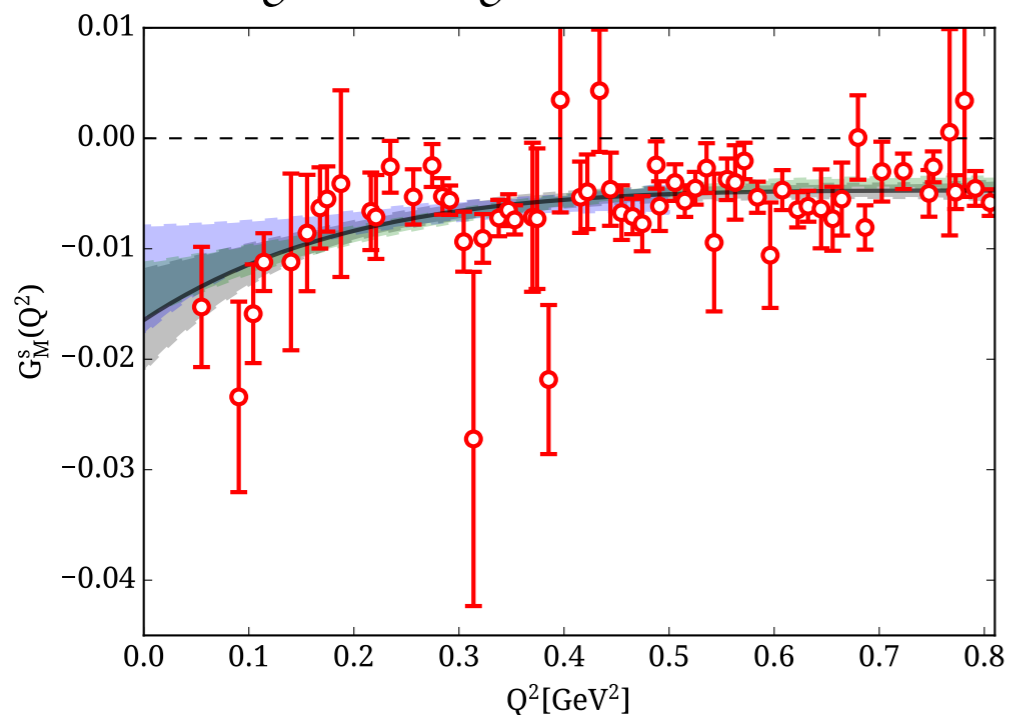
Strangeness of the nucleon

✳ Sea quark effects can be accurately determined for EM form factors → provide precise input to experiments

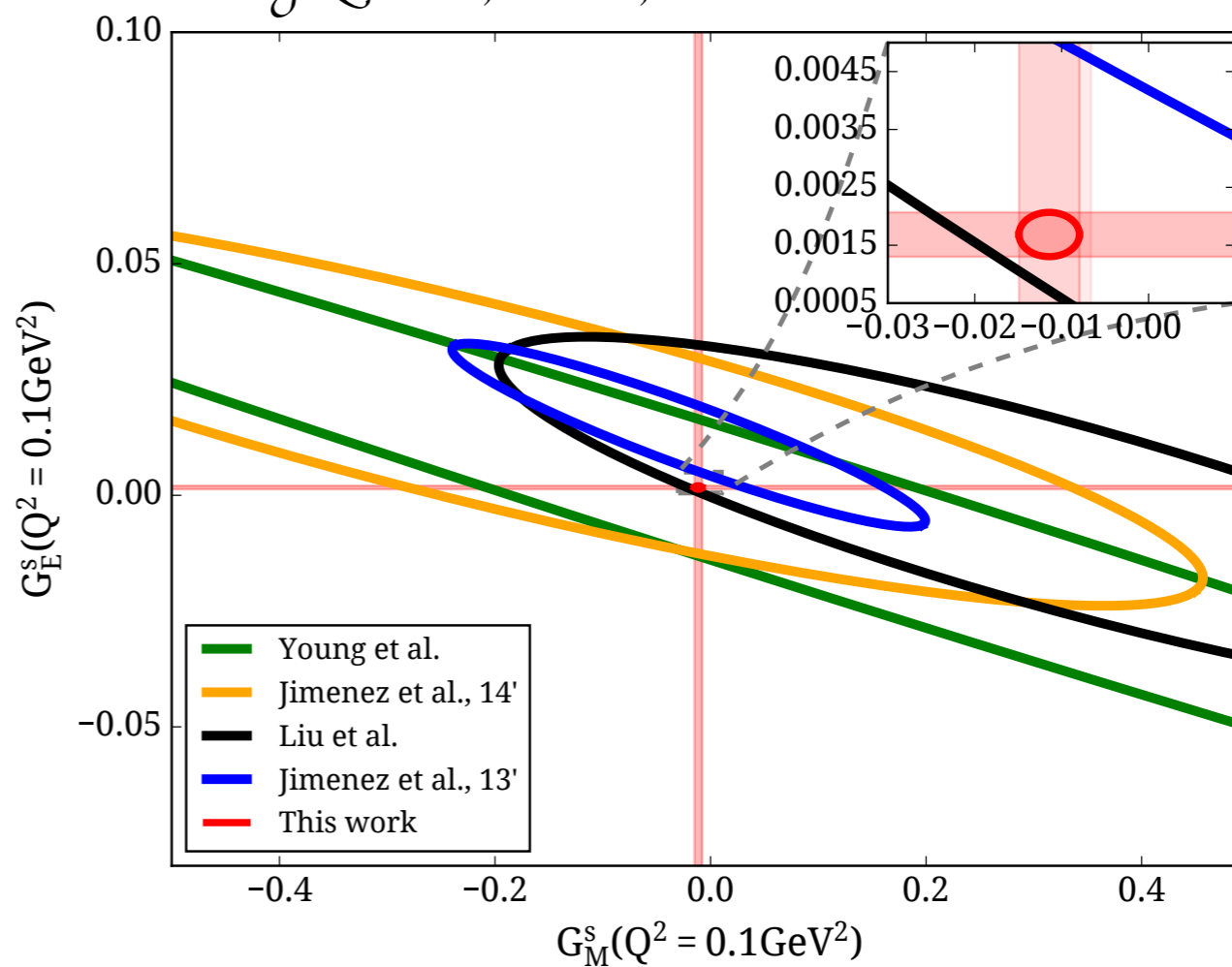
B64-ensemble: $64^3 \times 128$, $a \sim 0.08$ fm



Negative magnetic moment



*Significant input to experimental searches
e.g. Q-Weak, SolID, etc*



Axial and induced pseudoscalar form factors

Extract from lattice QCD

$$\langle N(p', s') | A_\mu | N(p, s) \rangle = \bar{u}_N(p', s') \left[\gamma_\mu G_A(Q^2) - \frac{Q_\mu}{2m_N} G_P(Q^2) \right] \gamma_5 u_N(p, s)$$

$$\langle N(p', s') | P_5 | N(p, s) \rangle = G_5(Q^2) \bar{u}_N(p', s') \gamma_5 u_N(p, s) \quad q^2 = -Q^2$$

✱ Check the PCAC : $\partial^\mu A_\mu = 2m_q P$, $m_q = m_u = m_d$

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

Goldberger-Treiman relation

✱ Relate to pion field: $G_5(Q^2) = \frac{F_\pi m_\pi^2}{m_q} \frac{G_{\pi NN}(Q^2)}{m_\pi^2 + Q^2}$

$$\rightarrow G_P(Q^2) = \frac{4m_N^2}{Q^2 + m_\pi^2} G_A(Q^2) \quad m_N G_A(Q^2) = F_\pi G_{\pi NN}(Q^2)$$

✱ At the pion pole we get the pion nucleon coupling: $g_{\pi NN} \equiv G_{\pi NN}(Q^2 = -m_\pi^2)$

$$\lim_{Q^2 \rightarrow -m_\pi^2} (Q^2 + m_\pi^2) G_P(Q^2) = 4m_N F_\pi g_{\pi NN}$$

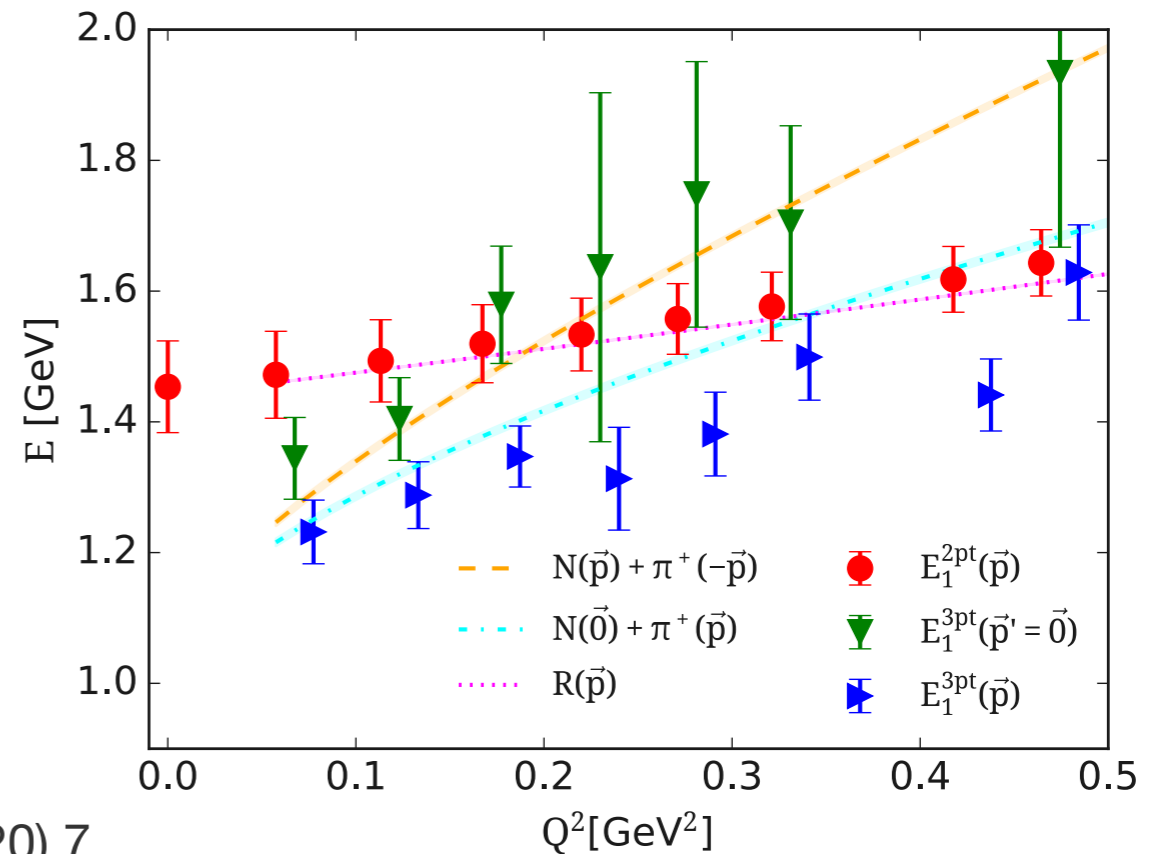
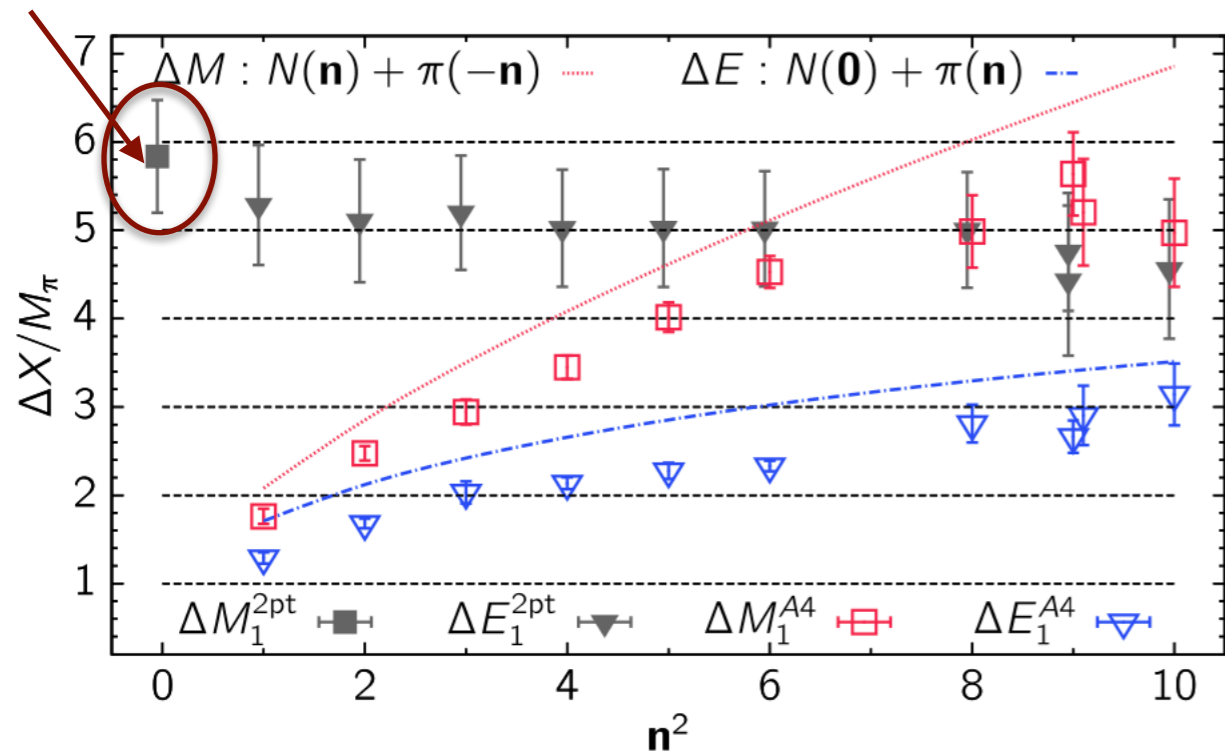
and $g_{\pi NN} = m_N G_A(-m_\pi^2) / F_\pi \xrightarrow{m_\pi \rightarrow 0} \frac{m_N}{F_\pi} g_A$

Analysis of excited states

We allow the first excited state to be different in the two- and three-point functions, O. Baer, *Phys. Rev. D* 99, 054506 (2019).

*Extract first excited state from the zero component of the axial-vector current

$\Delta M_1 \sim 800$ MeV

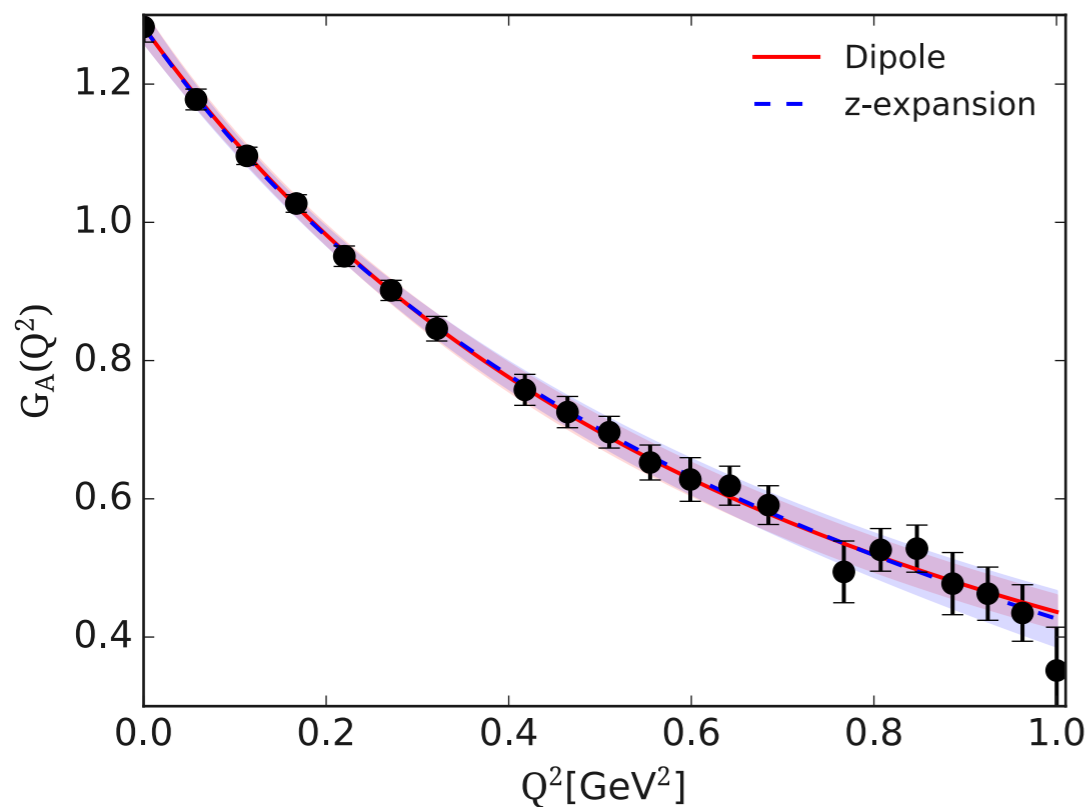


PNDME: Yong-Chull Jang et al., *Phys. Rev. Lett.* 124 (2020) 7, 072002, [1905.06470](https://arxiv.org/abs/1905.06470)

Axial form factor using the B64 ensemble

✱ Fit the Q^2 dependence using a dipole and z-expansion

$$G_A(Q^2) = \frac{g_A}{(1 + Q^2/m_A^2)^2} \quad \text{or} \quad G(Q^2) = \sum_{k=0}^{k_{\max}} a_k z^k(Q^2) \quad \text{and} \quad z(Q^2) = \frac{\sqrt{t_{\text{cut}} + Q^2} - \sqrt{t_{\text{cut}}}}{\sqrt{t_{\text{cut}} + Q^2} + \sqrt{t_{\text{cut}}}}$$

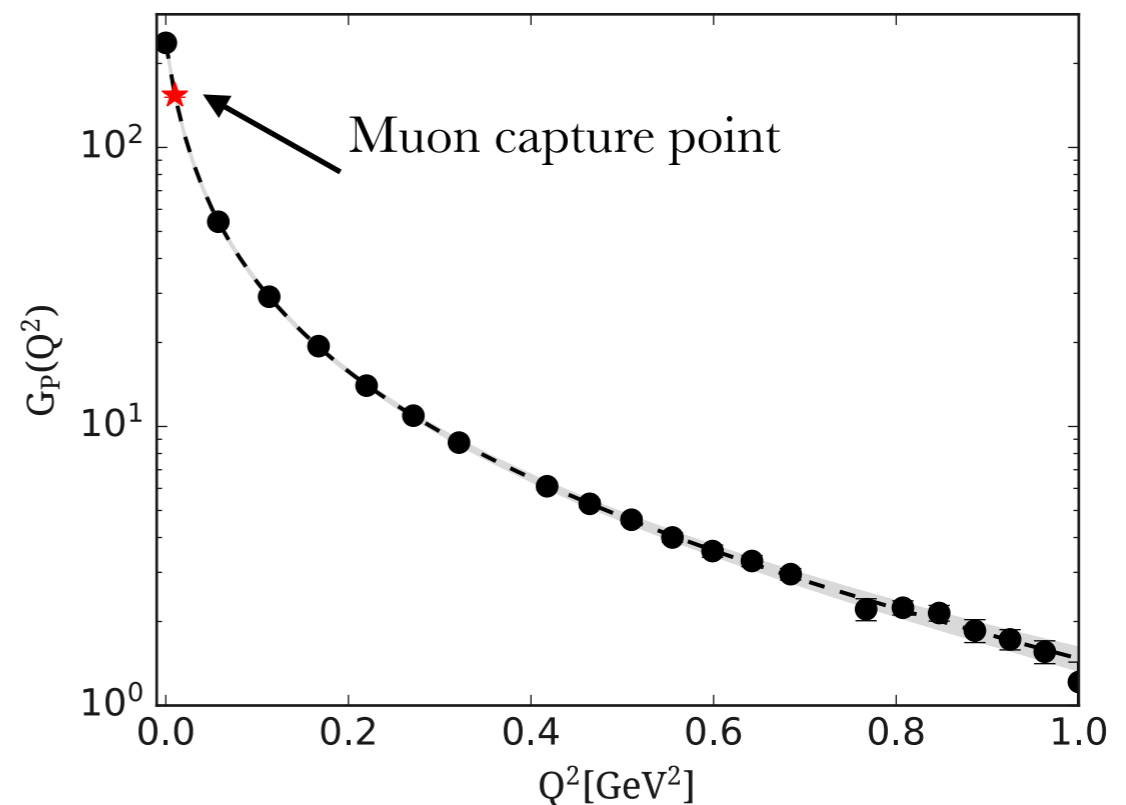


Using the z-expansion we find:

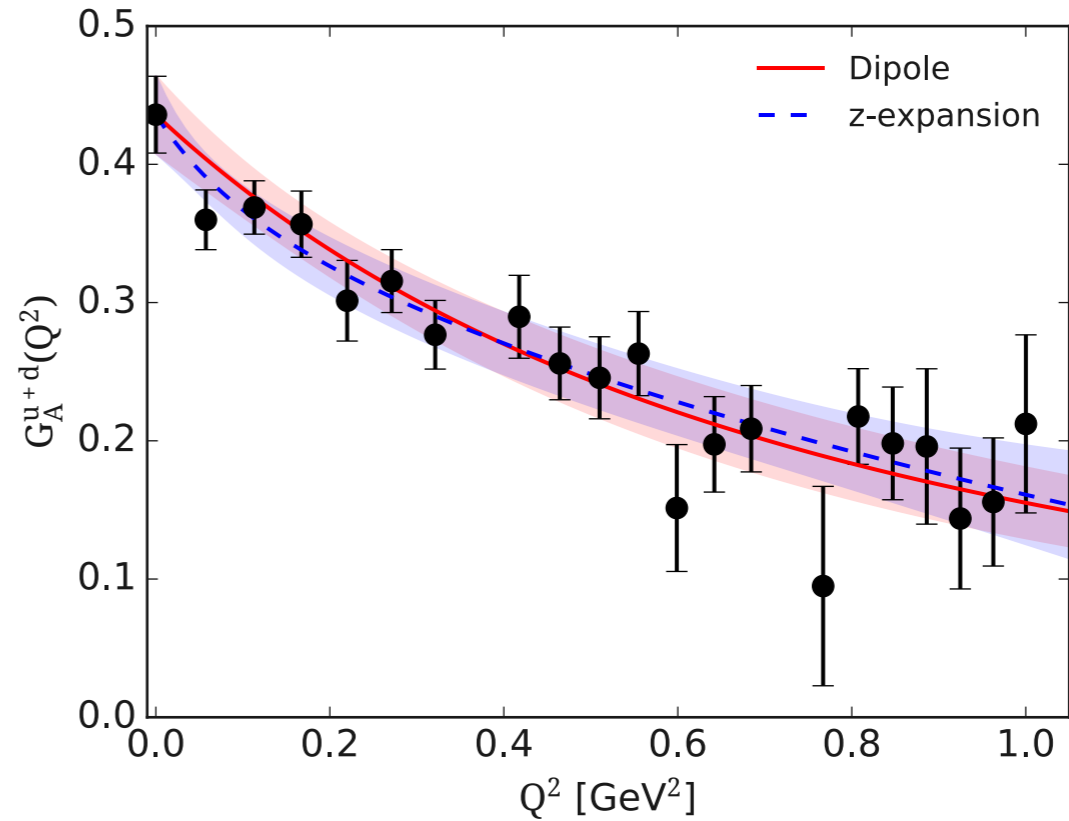
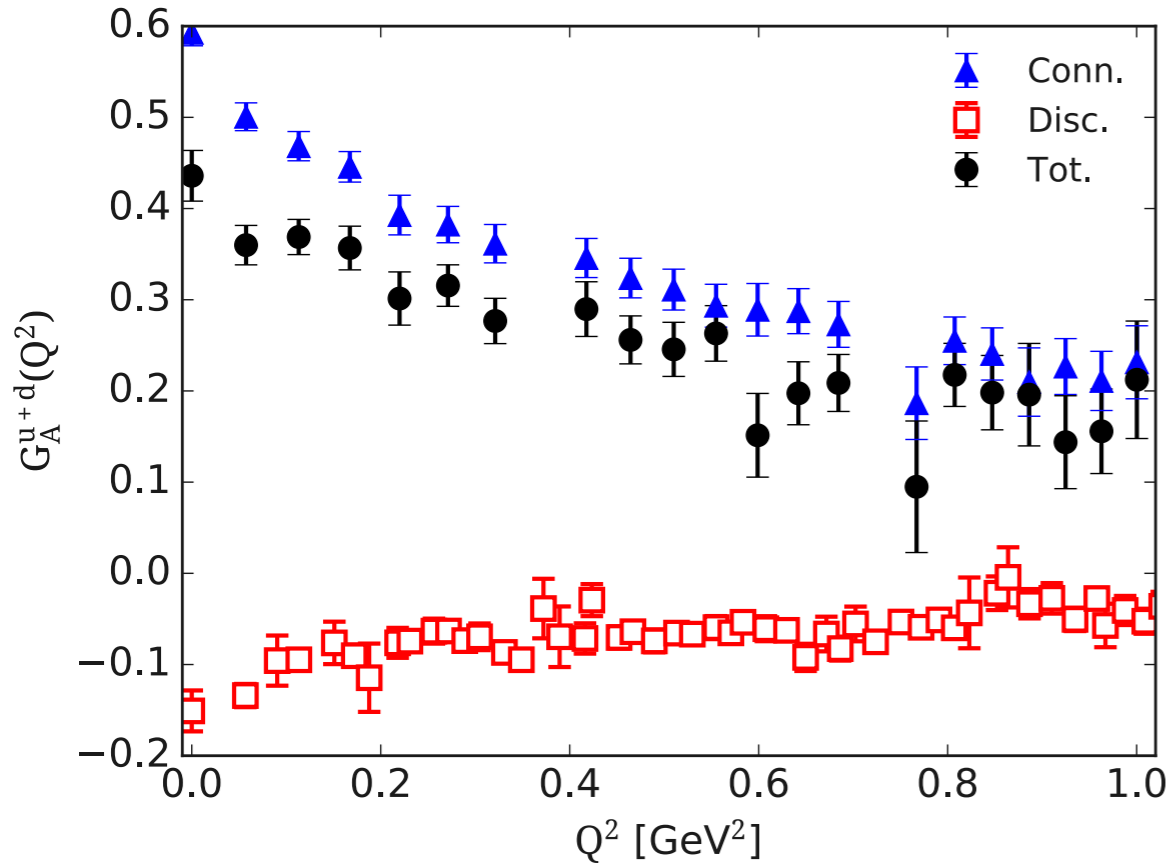
$$m_A = 1.169(72)(27) \text{ GeV}$$

$$\sqrt{\langle r_A \rangle^2} = 0.585(36)(14) \text{ fm}$$

Use PCAC to get G_P from G_A

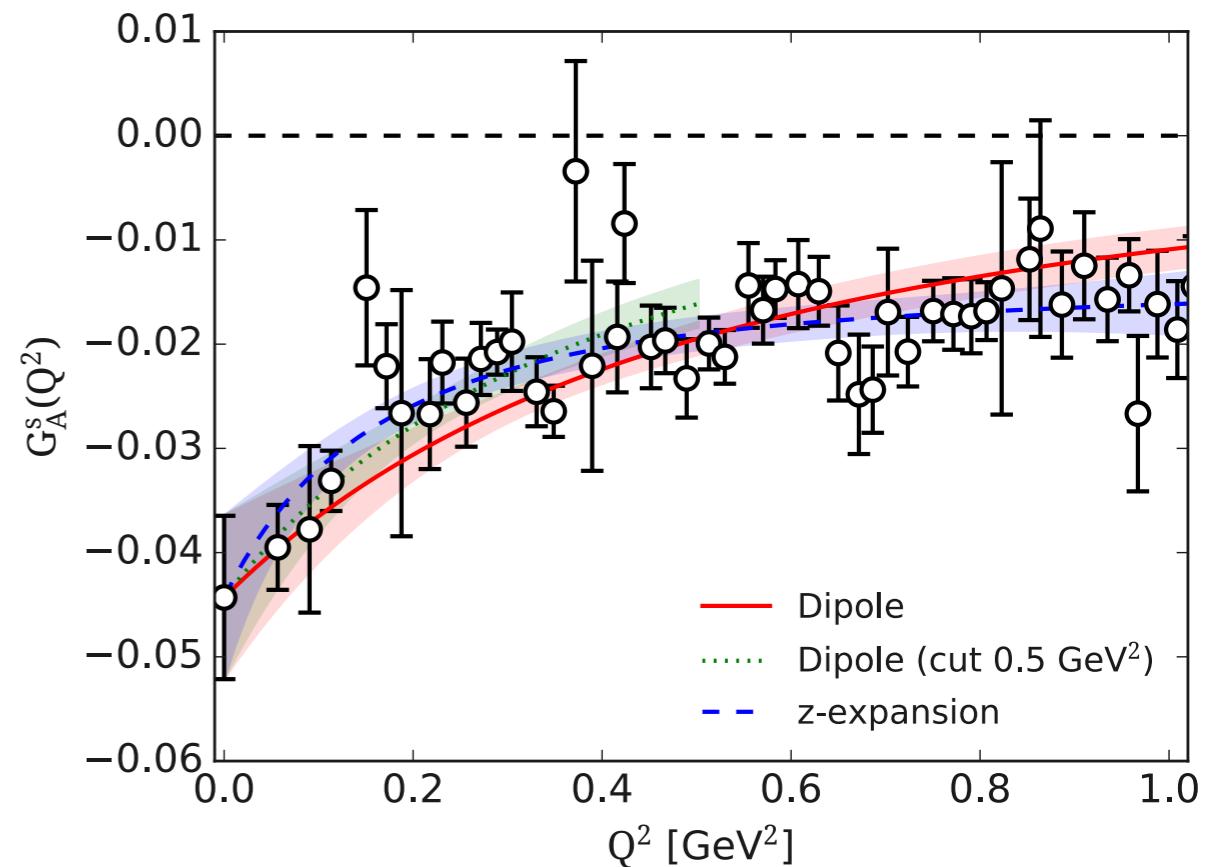


Quark flavour decomposition of G_A

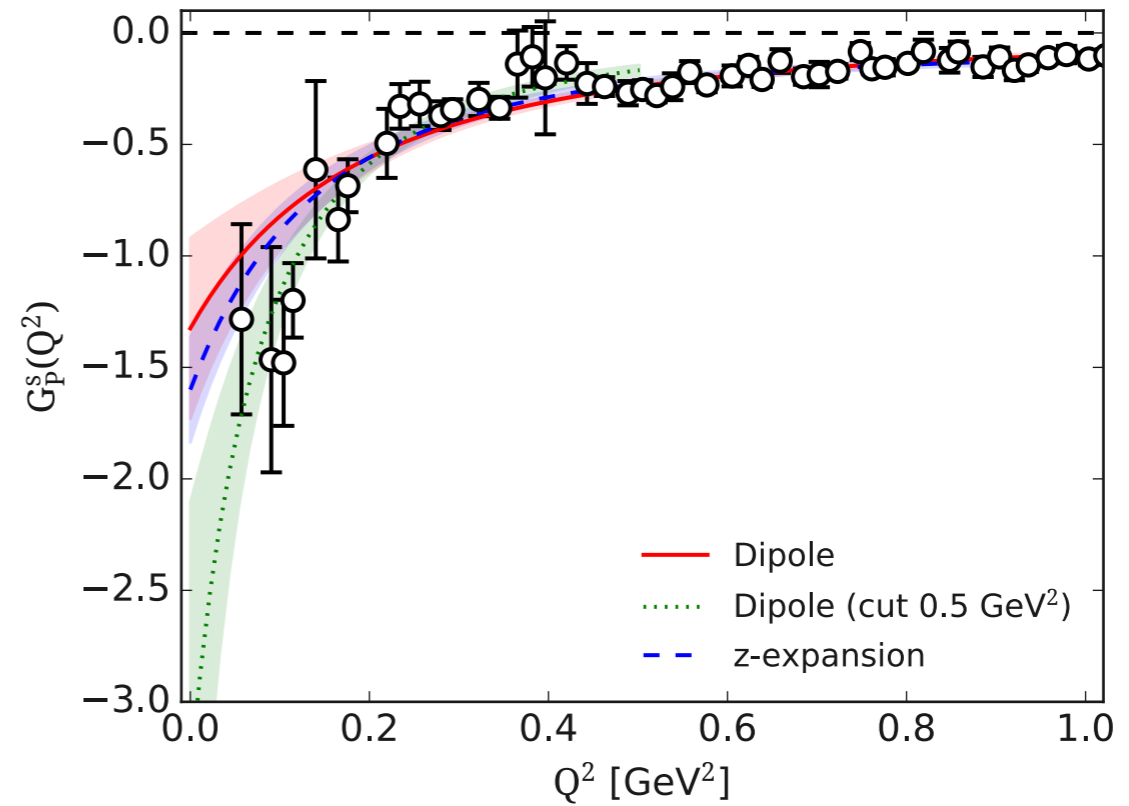
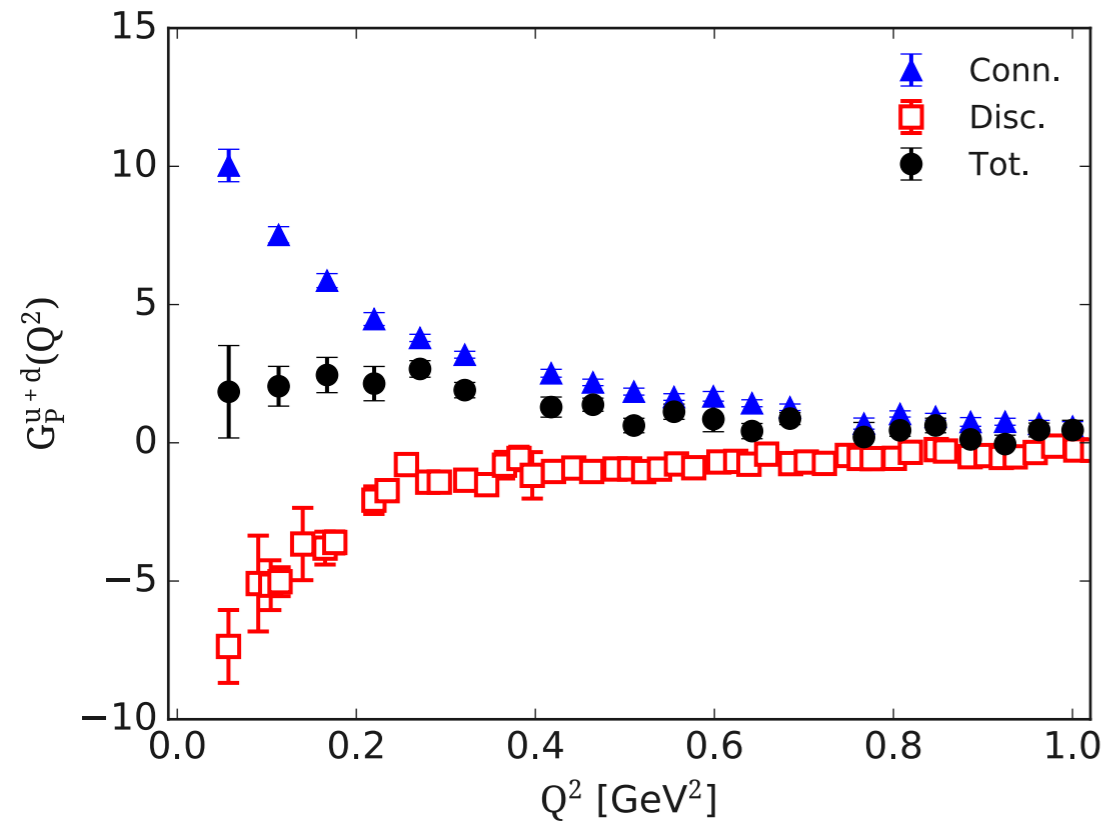


Contribution of disconnected diagrams

- Significant contribution of disconnected to u+d combination
- Negative disconnected contribution: subtracts from connected
- Good signal for strange contribution: clearly non-zero and negative



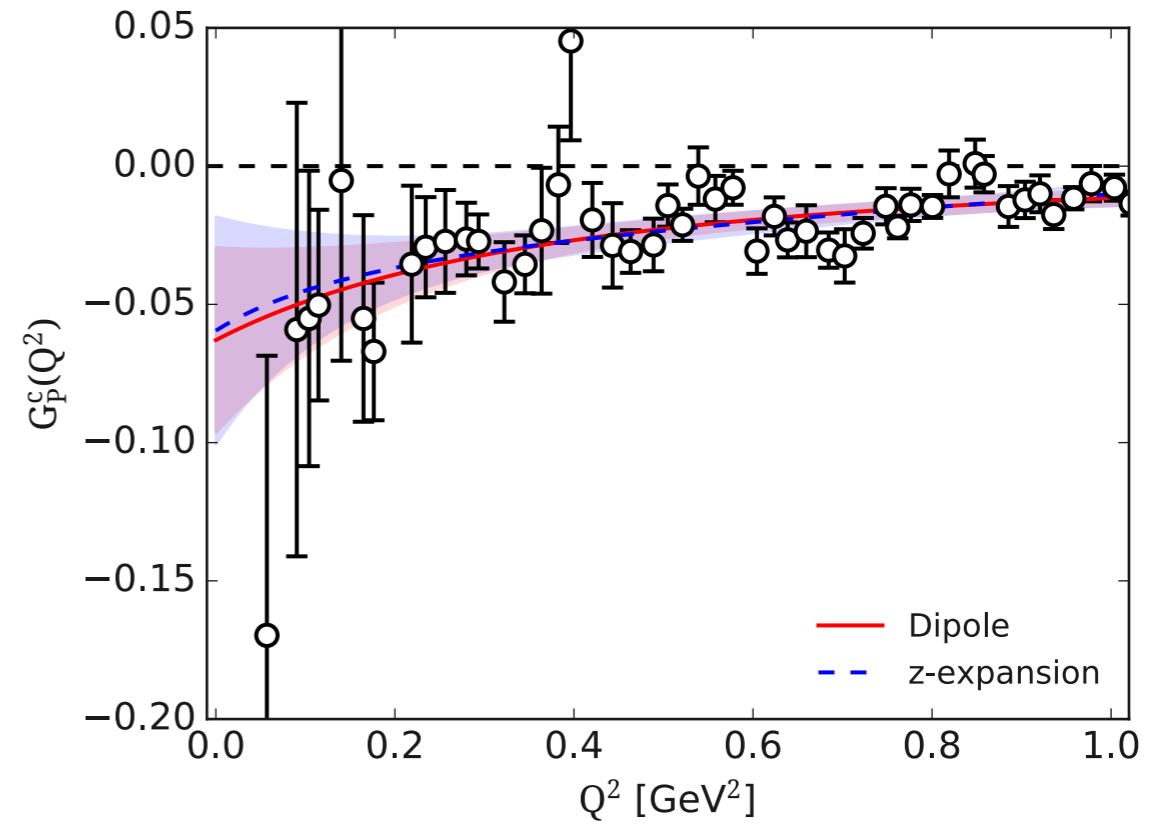
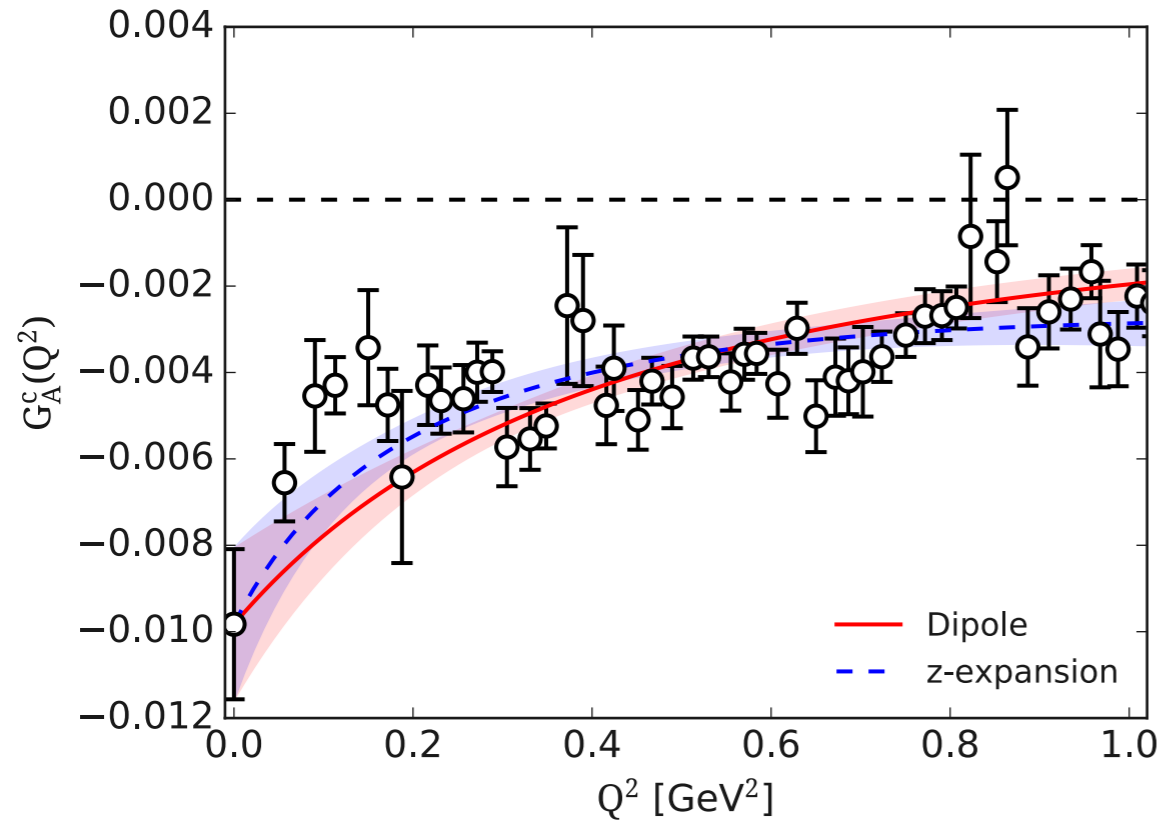
Quark flavour decomposition of G_P



Contribution of disconnected diagrams

- Significant contribution of disconnected to u+d combination
- Negative large disconnected contribution: subtracts from connected
- Large negative strange quark contribution

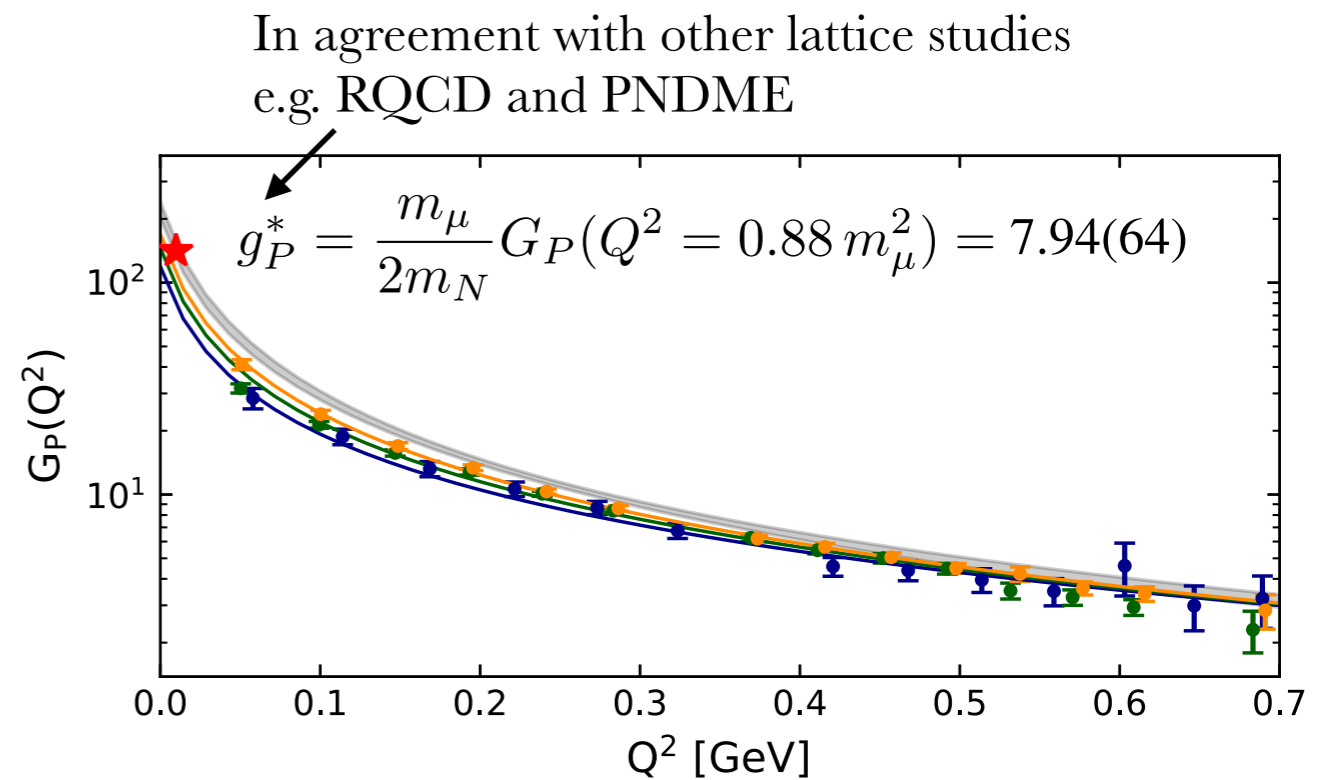
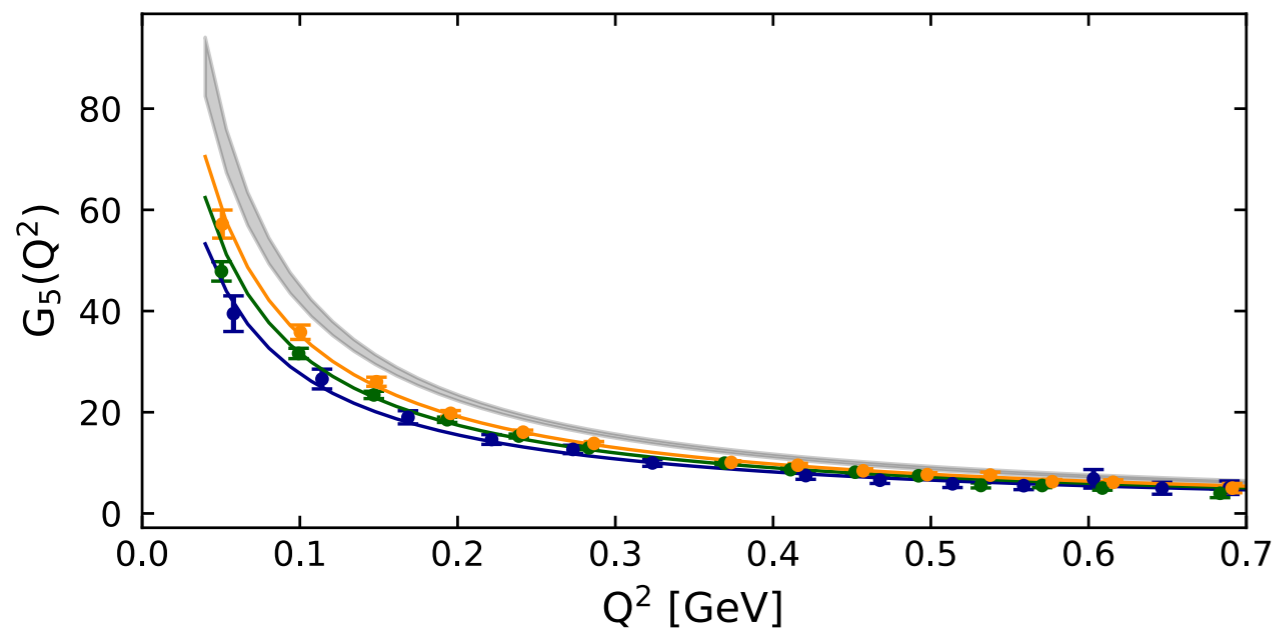
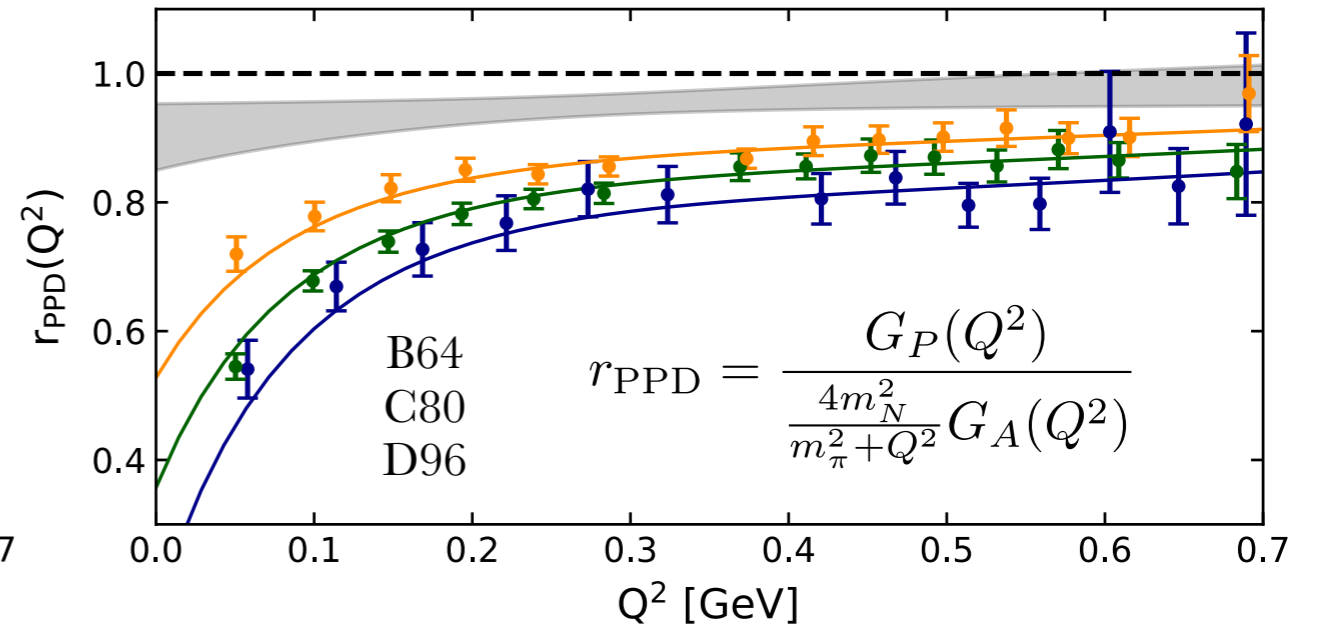
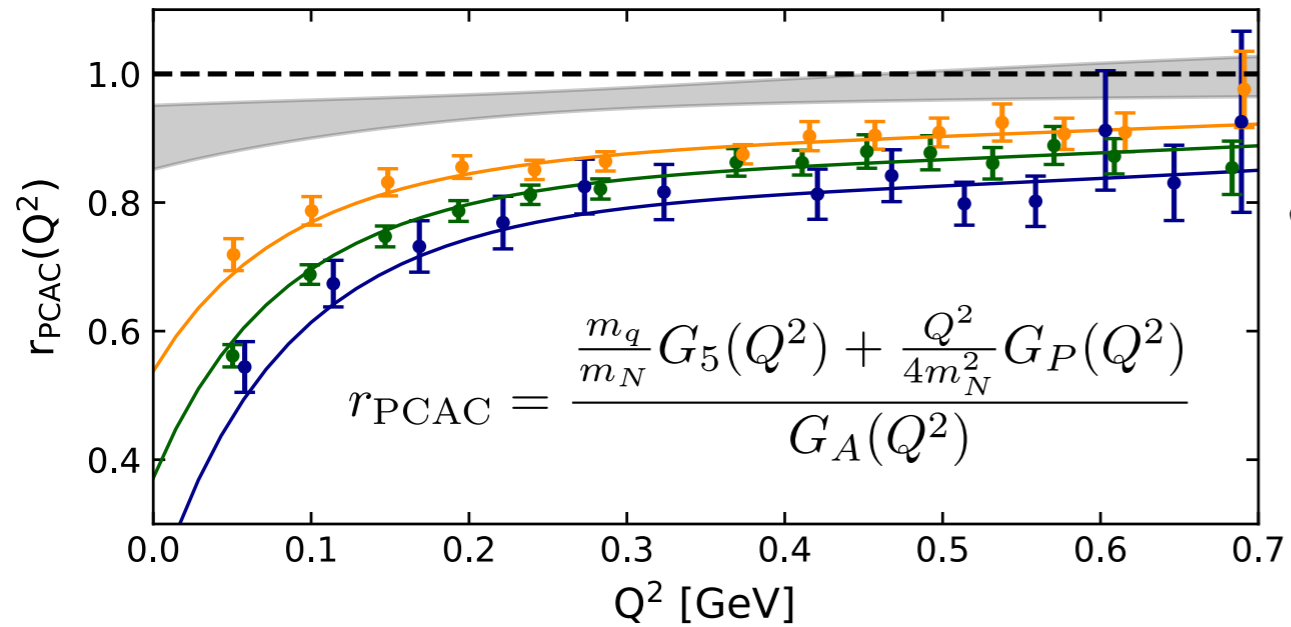
Charm quark contributions



✳ Clearly non-zero negative contributions for both axial form factors

(3) Sea quarks effects clearly seen on the form factors

PCAC and pion pole dominance (PPD) at the continuum limit



(4) Both PCAC and PPD are recovered in the continuum limit

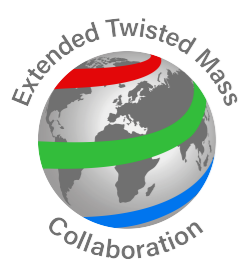
Conclusions

- (1) Lattice QCD results converge to the experimental values of e.g. nucleon axial charge, form factors, etc
- (2) A number of accurate results with controlled systematics on less known quantities provide valuable input for searches of new physics, e.g nucleon scalar and tensor charges including flavor diagonal, strangeness, ...
- (3) Lattice QCD reveals clearly strange and charm effects in the nucleon Direct computation of PDFs is a very active field
- (4) Continuum limit is important for recovering important relations
- (5) Same approaches can be used for other baryons and for non-diagonal matrix elements



Backup slides

Computational resources



Piz Daint, CSCS



JSC



HAWK, HLRS



SuperMUC, LRZ



Summit, OLCF

USA



Stampede, TACC



Marconi100, CINECA



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