

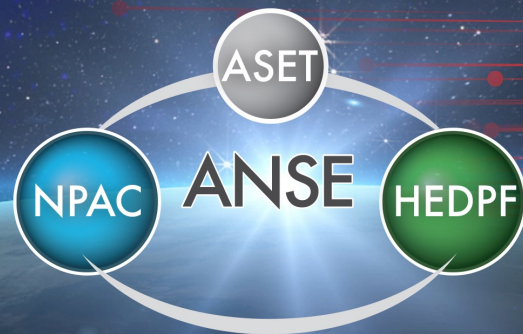
Nucleon charges and moments of PDFs from lattice QCD

Rajan Gupta

T-2, Theoretical Division

TMD Collaboration Meeting: June 17, 2022

LA-UR-22-25664



Abstract

I will review results for nucleon charges and moments of momentum fraction, helicity and transversity obtained from lattice QCD and discuss systematics using the results obtained by the LANL lattice QCD team as benchmarks.



PNDME and NME collaborations

- Tanmoy Bhattacharya (T-2)
- Vincenzo Cirigliano (T-2 → INT, UW)
- Rajan Gupta (T-2)
- Emanuele Mereghetti (T-2)
- Boram Yoon (CCS-7)
- Junsik Yoo (PD: 2022 May –)
- Yong-Chull Jang (PD: 2017-2018)
- Sungwoo Park (PD: 2018-2021)
- Santanu Mondal (PD: 2019-2021)
- Huey-Wen Lin (MSU)
- Balint Joo (ORNL)
- Frank Winter (Jlab)

References

- Charges: Gupta et al, PRD.98 (2018) 034503
- AFF: Gupta et al, PRD 96 (2017) 114503
- AFF: Jang et al, PRL 124 (2020) 072002
- VFF: Jang et al, PRD 100 (2020) 014507
- 2+1 clover: Park et al, PRD 105 (2022) 054505
- $\sigma_{\pi N}$ Gupta et al, PRL 127 (2021) 242002
- d_n from Θ -term Bhattacharya et al, PRD 103 (2021) 114507
- d_n from qEDM Gupta et al, PRD 98 (2018) 091501
- Moments Mondal et al, PRD 102 (2020) 054512
- Moments Mondal et al, JHEP 04 (2021) 044
- Proton spin Lin et al, PRD 98 (2018) 094512



Lattice QCD is the best-known method to calculate non-perturbative properties of QCD (quarks and gluons)

- Properties of QCD and hadrons
- QCD corrections to weak and electromagnetic processes
- QCD corrections to beyond the standard model processes

PNDME Collaboration:

Thirteen 2+1+1-flavor HISQ ensembles = clover-on-HISQ formulation

NME Collaboration:

Thirteen 2+1-flavor clover ensembles = clover-on-clover formulation



Rich Landscape of LQCD calculations

HEP

ϵ, ϵ' in kaon
CP violation

s, c, b decay
form factors

$g-2$

α_s , quark
masses

NP

Nucleon structure,
form factors

Matrix elements
within Nuclei

Parton distribution functions

PDFs

Hadron
Spectroscopy

Physics objectives

Charges

$g_A, g_S, g_T, \sigma_{\pi N}, \sigma_S$

Axial & EM
form factors

Neutron electric
dipole moment

nEDM

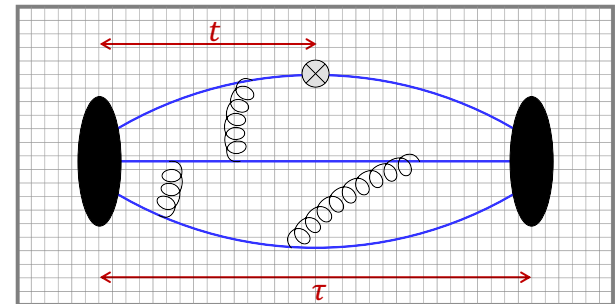
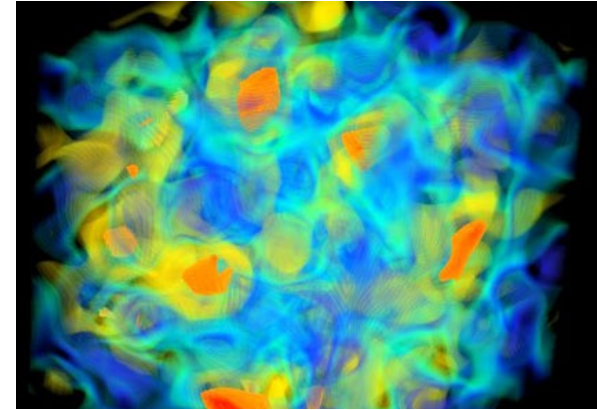
Neutrinoless double
beta decay

$0\nu\beta\beta$

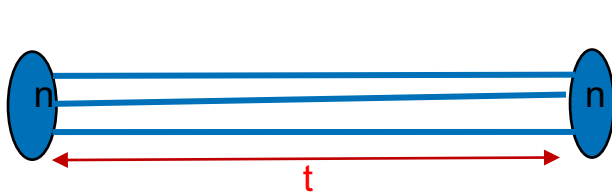


What simulations of LQCD provide

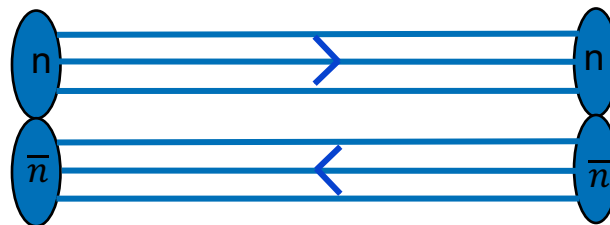
- The quantum vacuum of QCD
 - ensemble of gauge configurations
- Input hadrons & interactions as external probes
 - N-point correlation functions
- Quantum wavefunctions of hadronic states
 - Matrix elements: $\langle N(p_f) | O(Q^2) | N(p_i) \rangle$



Spectrum from the 2-point function Γ^{2pt}



Signal in Γ^{2pt} : $e^{-E_N t}$



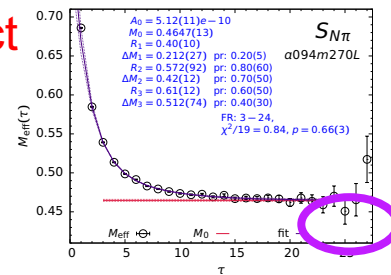
Variance: $e^{-3E_\pi t}$

$$\Gamma^2(t) = |A_0|^2 e^{-M_0 t} + |A_1|^2 e^{-M_1 t} + |A_2|^2 e^{-M_2 t} + |A_3|^2 e^{-M_3 t} + \dots$$

Fit the data for $\Gamma^{2pt}(t)$ versus t to extract

M_0, M_1, \dots masses of the ground & excited states

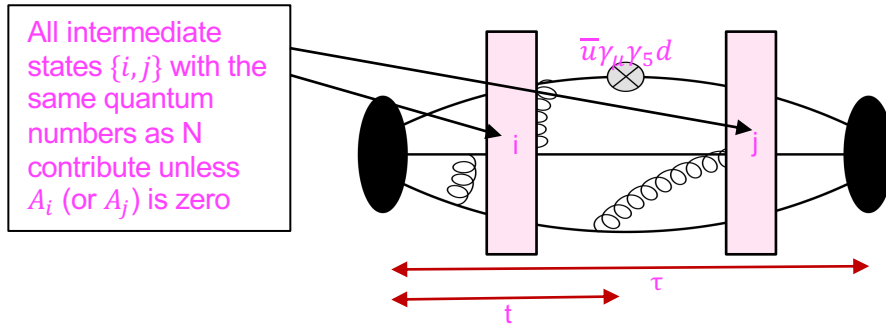
A_0, A_1, \dots corresponding amplitudes



- The signal degrades exponentially $e^{-(M_N - 1.5M_\pi)t}$
- Need large t to “kill” states with small mass gap: $\Delta M_{N\pi} \sim 300\text{MeV}$



Calculation of nucleon 3-point functions using LQCD is mature, but



All intermediate states $\{i, j\}$ with the same quantum numbers as N contribute unless A_i (or A_j) is zero

Radial excited States:

$N(1440), N(1710)$

Towers of multihadrons states

$N(\vec{k})\pi(-\vec{k}) > 1200 \text{ MeV}$

$N(0)\pi(\vec{k})\pi(-\vec{k}) > 1200 \text{ MeV}$

Ground state properties (energy, amplitudes, ME) extracted from 2- and 3-point function using fits to the spectral decomposition

$$\Gamma^{2pt}(\tau) = \sum_i |A_i|^2 e^{-E_i \tau}$$

$$\Gamma_0^{3pt}(t, \tau) = \sum_{i,j} A_i^* A_j \underbrace{\langle i | O | j \rangle}_{\text{Extract } \langle 0 | O | 0 \rangle} e^{-E_i t - E_j (\tau - t)}$$

Extract $\langle 0 | O | 0 \rangle$

Including multihadron states in fits remains a challenge



LQCD Methodology, Tools, Challenges

- Generate gauge configurations
- Create states and isolate ground state wavefunctions ($e^{-E_i\tau}$)
- Formulate operators that best probe the physics
 - Low energy effective operators encapsulating SM & BSM physics
 - Examples: Axial, scalar, tensor and vector quark bilinears ($O = \bar{q} \Gamma_i q$), ...
- Calculate matrix elements: $\langle N(p_f) | O(Q^2) | N(p_i) \rangle$
- Signal to noise ratio degrades exponentially $e^{-(M_N - 1.5M_\pi)\tau}$
- Need to control large excited state contamination in all NME



Neutron Electric Dipole Moment (nEDM) d_n

- 5 kinds of CPV operators: Θ -term, qEDM, chromoEDM, Weinberg, 4-fermion
- $d_n = \sum_{O_i} \epsilon_i X_i$ where the sum is over all CPV operators O_i with coupling ϵ_i
- X_i are the CPV part of matrix elements of O_i within the neutron ground state
- Measure d_n and calculate X_i using LQCD \Rightarrow constrain ϵ_i (BSM models)

If $d_n \gtrsim 10^{-28} e \text{ cm} \rightarrow$ CP violation in quark sector large enough for many BSM to remain viable.

Baryogenesis a viable mechanism for observed matter-antimatter asymmetry in the universe.

Need X_i to constrain BSM theories



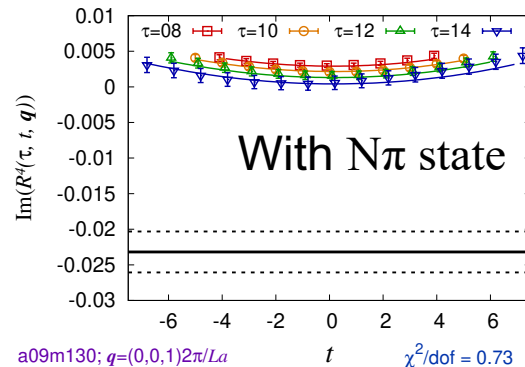
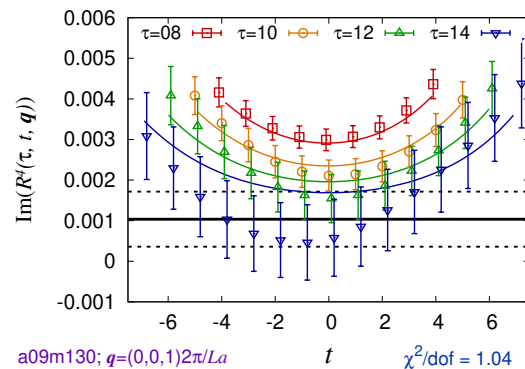
Contribution of the Θ -term to neutron EDM

- $L_\Theta = \Theta \frac{iG_{\mu\nu}^a \tilde{G}_{\mu\nu}^a}{32\pi^2}$ is a D=4 interaction that violates P and T (CP if CPT holds)
- This D=4 term is allowed in the standard model
- $\Theta \sim 10^{-10}$ (from $d_n \leq 1.8 \times 10^{-26}$ e cm) is unnaturally small
- Axion: solution proposed to explain this small coupling

Lattice calculation of X_Θ : $d_n = \Theta X_\Theta \equiv \Theta \left\langle N \left| \frac{L_\Theta}{\Theta} \right| N \right\rangle_{CPV}$

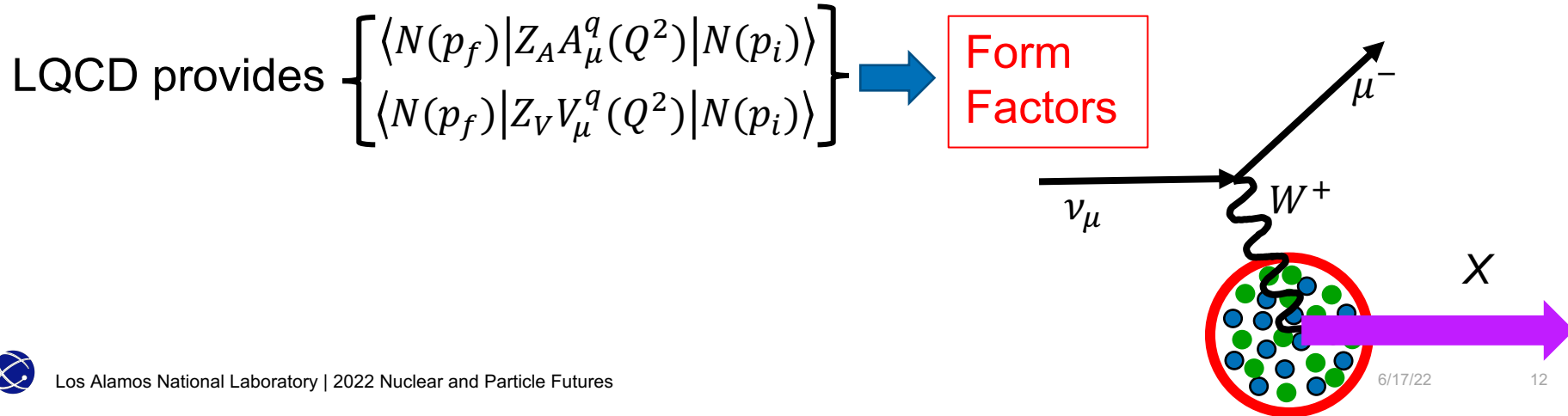
- Value of X_Θ is small and signal is poor
- χ PT indicates that $N\pi$ states contribute
- Result for d_n is very sensitive to excited states included in the analysis. Much larger d_n with $N\pi$ states!!

No robust result from LQCD yet: PRD 103 (2021) 114507



Axial vector form factors

- Neutrino oscillation experiments need electromagnetic and axial vector form factors for the calculation of neutrino flux and cross-section @ DUNE, T2K, ...
- Electromagnetic form factors well measured from electron scattering
- LQCD best method to calculate axial vector form factors of nucleons
- Nuclear corrections being calculated by many body nuclear theory



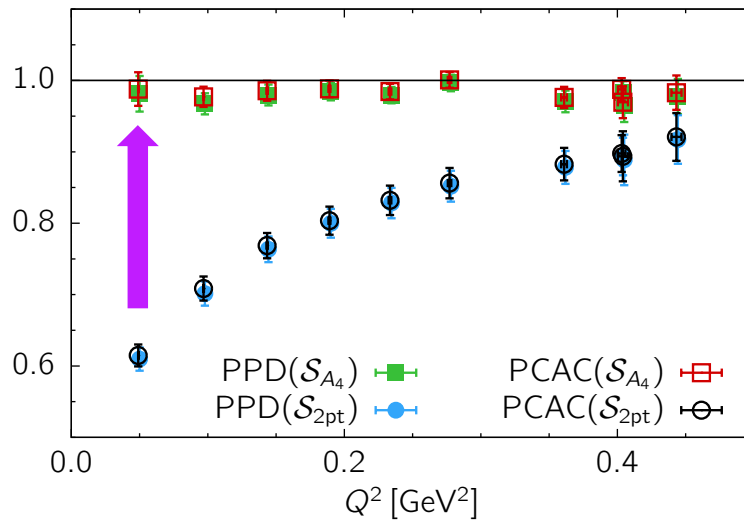
2017→2019: Reconcile AFF with PCAC and PPD

Gupta et al, PhysRevD.96.114503 → Jang et al, PRL 124 (2020) 072002

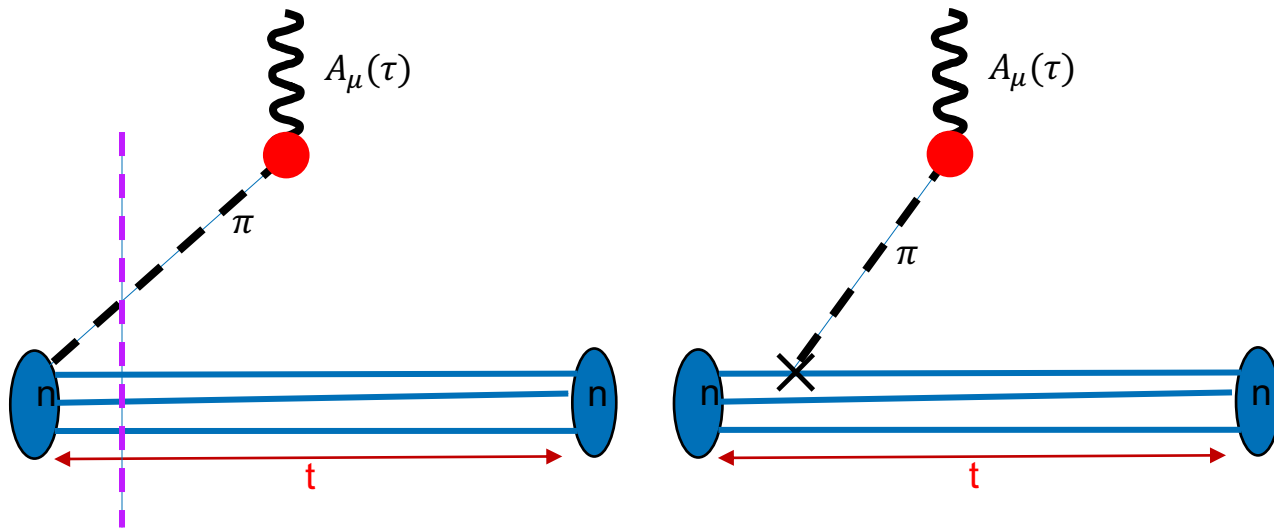
On including low mass $N_{p=0}\pi_p$ and $N_p\pi_{-p}$ excited states neglected in previous works, FF satisfy PCAC and PPD at ~5%

$$\frac{\hat{m}G_P}{M_N G_A} + \frac{Q^2 \tilde{G}_P}{4M_N^2 G_A} = 1$$

$$\frac{Q^2 + M_\pi^2}{4M_N^2} \frac{\tilde{G}_P(Q^2)}{G_A(Q^2)} = 1$$



χ_{PT} : $N\pi$ state coupling large in the axial channel



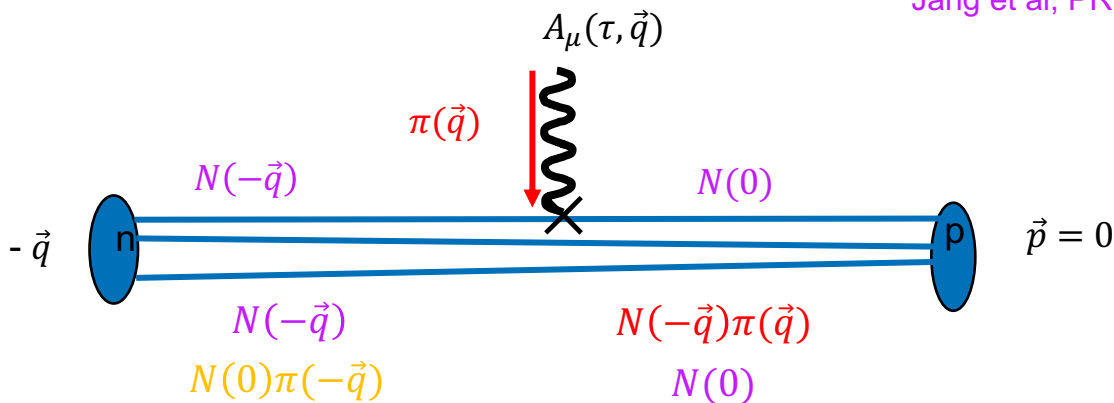
Enhanced coupling to $N\pi$ state: Since the pion is light, the vertex \bullet can be anywhere in the lattice 3-volume

Oliver Bär: Phys. Rev. D 99, 054506 (2019), Phys. Rev. D 100, 054507 (2019)

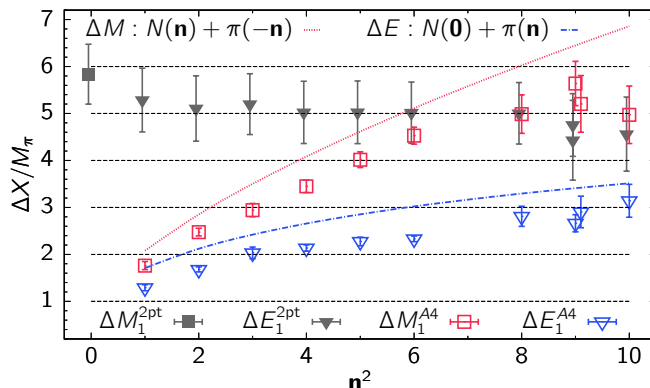


$N\pi$ state in the axial channel

Jang et al, PRL 124 (2020) 072002



Mass gaps extracted from fits match the above picture



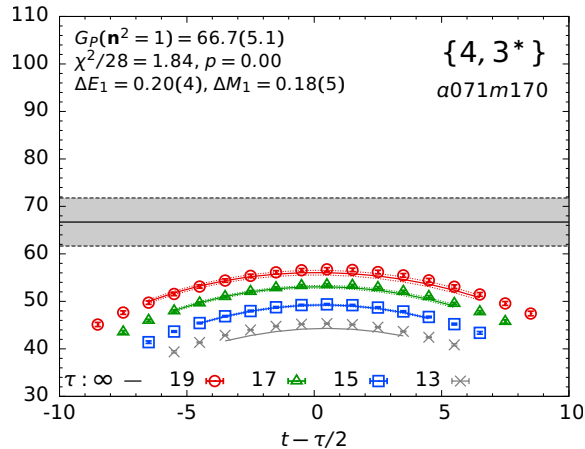
ΔM_1^{A4} and ΔE_1^{A4} are outputs of 2-state fit and not driven by priors



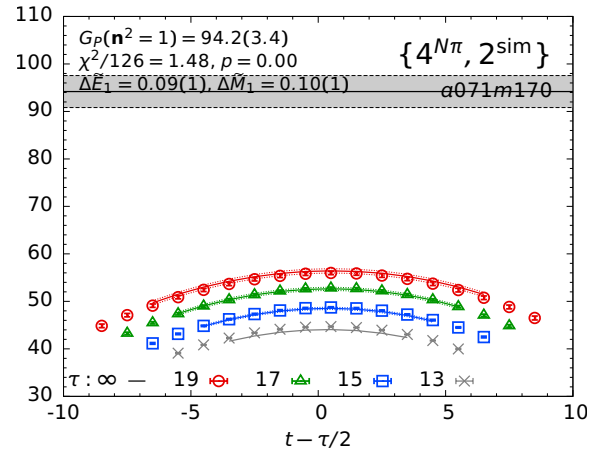
How large is the “ $N\pi$ ” effect?

Output of a simultaneous fit to $\langle A_i \rangle, \langle A_4 \rangle, \langle P \rangle$ (called $\{4^{N\pi}, 2^{sim}\}$ fit) increases the form factors by:

$$\left[\begin{array}{l} G_A \sim 5 \% \\ \tilde{G}_P \sim 35 \% \\ G_P \sim 35 \% \end{array} \right.$$



Standard 3-state fit to $\langle P \rangle$



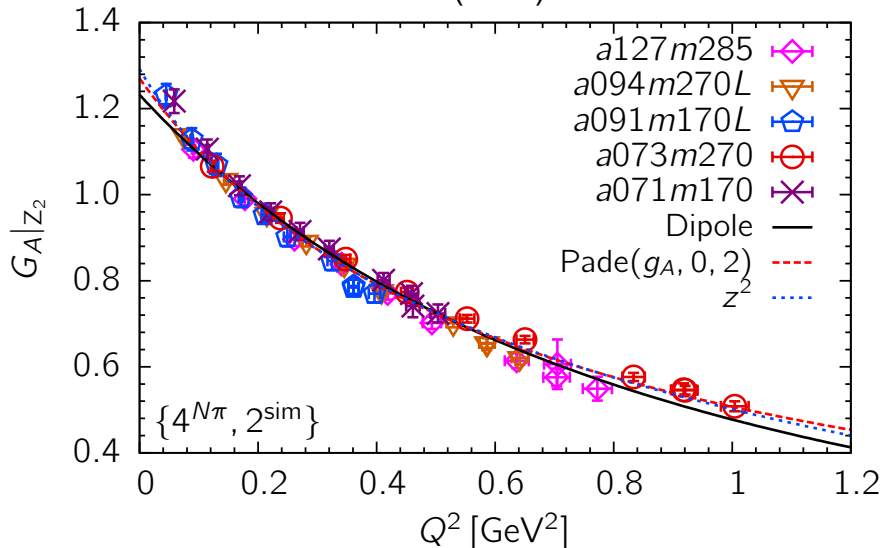
Simultaneous 2-state to $\langle A_i \rangle, \langle A_4 \rangle, \langle P \rangle$ correlators



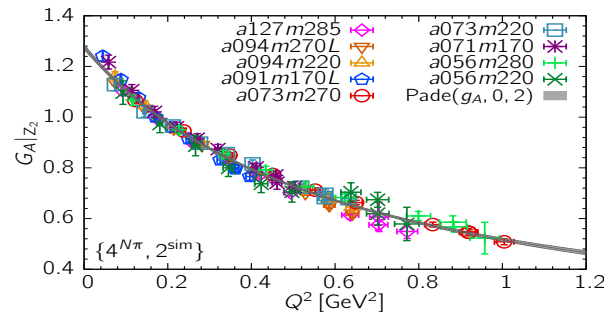
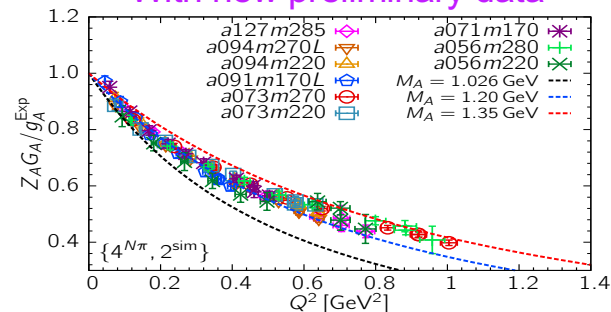
Axial Form Factor: $G_A(Q^2)$

PRD 105 (2022) 054505

PRD 105 (2022) 054505



With new preliminary data



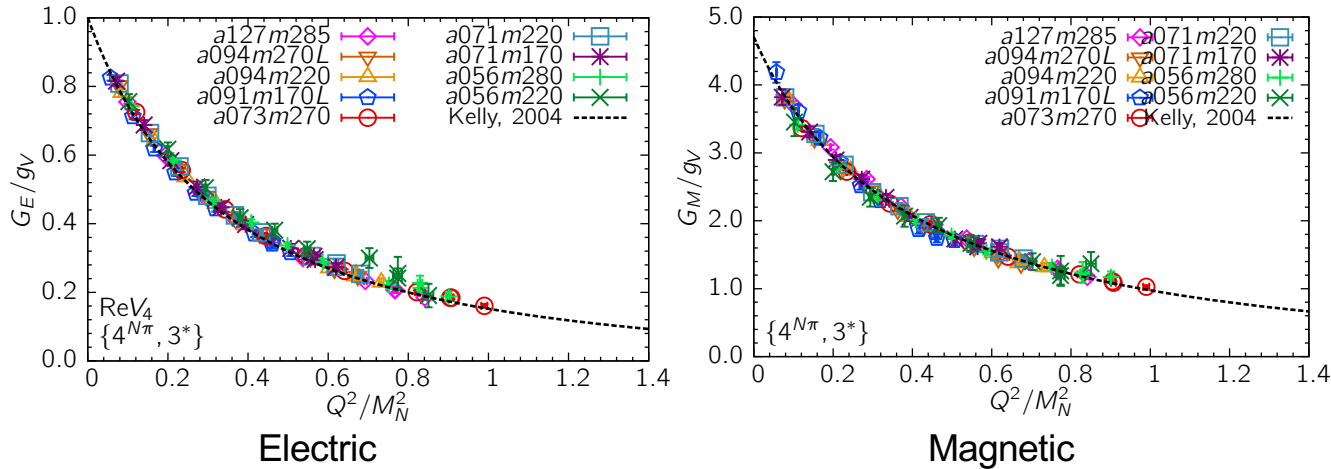
$$G_A(Q^2) = \frac{g_A = 1.270(11)}{1 + 5.36(20) \frac{Q^2}{4M_N^2} - 0.22(81) \left(\frac{Q^2}{4M_N^2}\right)^2}$$

$$G_A(Q^2) = \frac{g_A = 1.277(9)}{1 + 5.47(20) \frac{Q^2}{4M_N^2} - 1.02(71) \left(\frac{Q^2}{4M_N^2}\right)^2}$$

$$\langle r_A^2 \rangle = 0.361(13) \text{ fm}^2$$



Electric & Magnetic FF with new data



- The extraction of electric and magnetic form factors is insensitive to the details of the excited states
- Vector meson dominance $\rightarrow N\pi\pi$ state should contribute (some evidence)
- The form factors do not show significant dependence on the lattice spacing or the quark mass
- Good agreement with the Kelly curve. *Validates the lattice methodology*
- Improve precision and get data over larger range of parameter values



The pion-nucleon sigma term

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

- Fundamental parameter of QCD that quantifies the amount of the nucleon mass generated by u and d quarks.
- g_S^2 : enters in cross-section of dark matter with nucleons
- Important input in the search of BSM physics

χ PT analysis shows $N(\vec{k})\pi(-\vec{k})$ and $N(\mathbf{0})\pi(\vec{k})\pi(-\vec{k})$ states give significant contributions.

Phenomenology: coupling of scalar operator to $\pi\pi$ is large

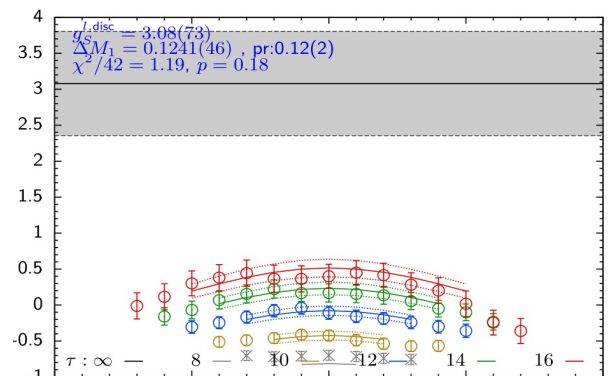
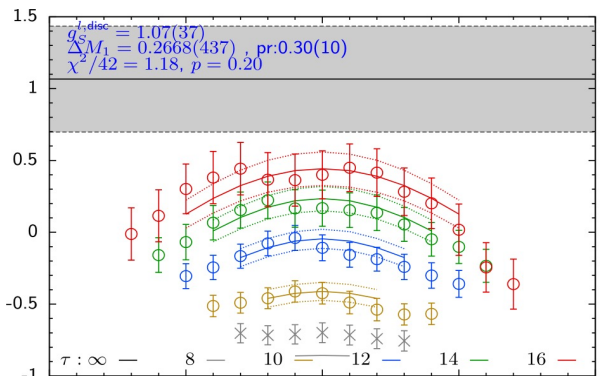


Excited-state effects large and very sensitive to $N\pi / N\pi\pi$ states

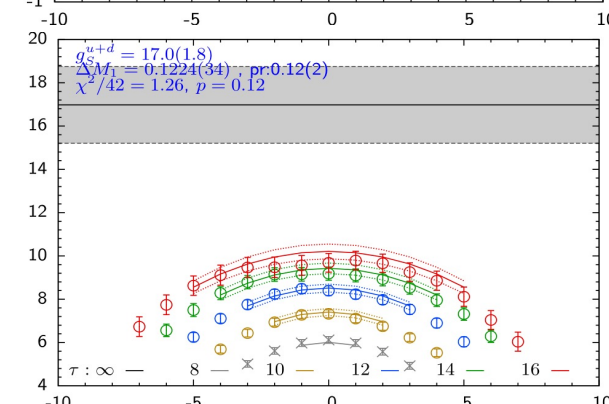
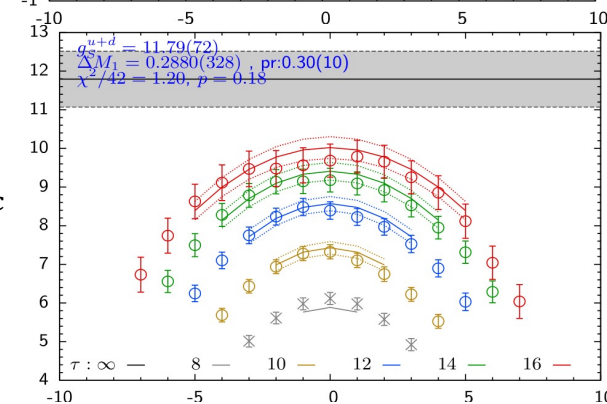
Fits without $N\pi/N\pi\pi$ ($M_1 \approx 1.6$ GeV)

with $N\pi / N\pi\pi$ ($M_1 \approx 1.2$ GeV)

$g_S^{l, disc}$



$$g_S^{u+d} = g_S^{u+d, conn} + 2g_S^{l, disc}$$



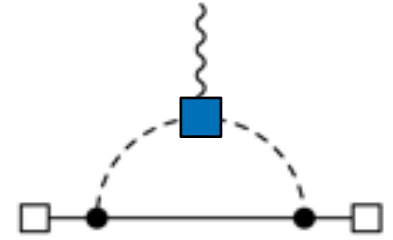
$\sigma_{\pi N} = m_l g_S^{u+d} \sim 40$ MeV

$\sigma_{\pi N} = m_l g_S^{u+d} \sim 60$ MeV



χ PT and excited states

- Leading corrections come from pion loops.
- Loops that originate or end at sources are ESC. These can be removed by a pure nucleon source.
- Loops that originate on the nucleon line give rise to both: corrections to the physical result and excited state contributions (from pions going on-shell in Minkowski)
- The latter are suppressed exponentially by the mass gap



Unless there are large cancellations, loops effects should be considered in both

- in removing excited state contamination
- in the chiral fits to the data to get results at $M_\pi = 135$ MeV



Resolved Tension Between Lattice and Phenomenology

FLAG Reports 2019, 2021:

- Previous Lattice results ~ 40 MeV
- Phenomenology favors ~ 60 MeV

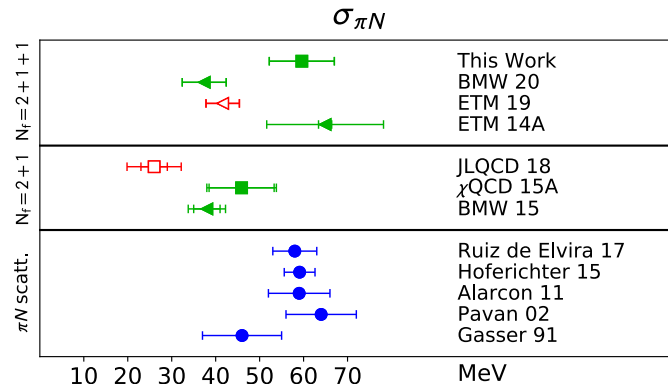
Recent results

BMW (arXiv:2007.03319) $\sigma_{\pi N} = 37.4(5.1)$ MeV (FH)

ETM (PRD **102**, 054517) $\sigma_{\pi N} = 41.6(3.8)$ MeV (Direct)

LANL Results: PRL 127 (2021) 242002

- Without including $N(\vec{k})\pi(-\vec{k})$ and $N(\mathbf{0})\pi(\vec{k})\pi(-\vec{k})$ states: $= 41.9 (4.9)$ MeV
- Including $N(\vec{k})\pi(-\vec{k})$ and $N(\mathbf{0})\pi(\vec{k})\pi(-\vec{k})$ states: $= 59.7 (7.3)$ MeV



quark contribution to proton spin

gauge invariant decomposition of the proton spin is given by (X. Ji, PRL 78 (1997) 610)

$$\frac{1}{2} = \sum_{\{u,d,s,c\}} \left(\frac{1}{2} \Delta q + L_q \right) + J_g$$

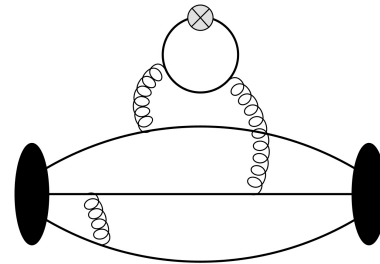
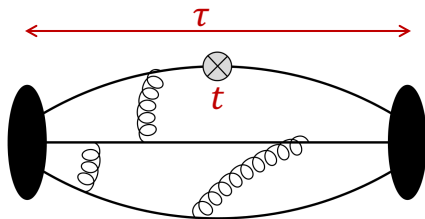
$$S_P^q = \sum_q S_q \equiv \sum_q \frac{\Delta q}{2} \equiv 0.5 \sum_q g_A^q \quad g_A^q = \langle N(p_i) | Z_A A_\mu^q(0) | N(p_i) \rangle$$

- These calculations are hard because we need to sum the contribution of

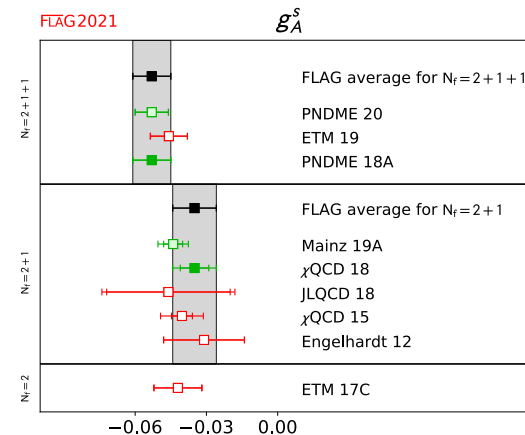
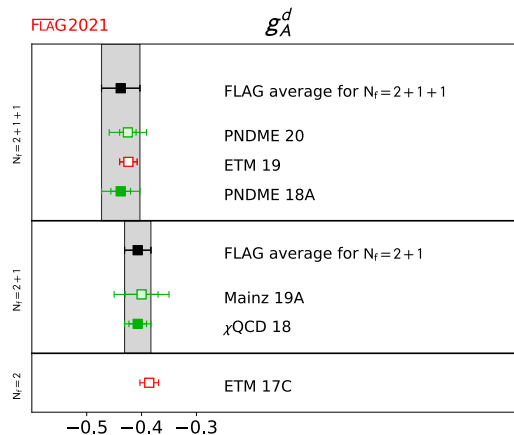
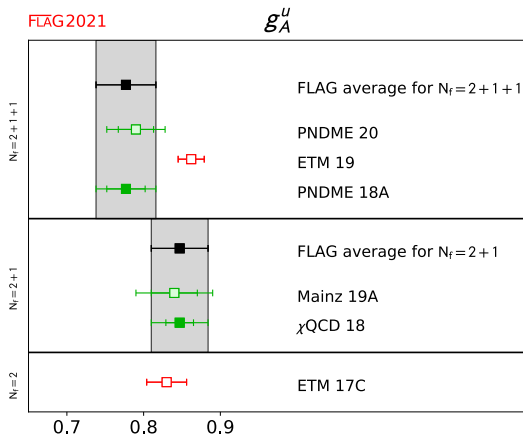
connected

+

disconnected diagrams



Compass result $0.13 \leq \sum_q S_q \equiv 0.5 \sum_q g_A^q \leq 0.18$



LANL (PNDME) result:

$$0.5 \sum_q g_A^q = (0.777(39) - 0.438(35) - 0.053(8))/2 = 0.143(31)(36)$$



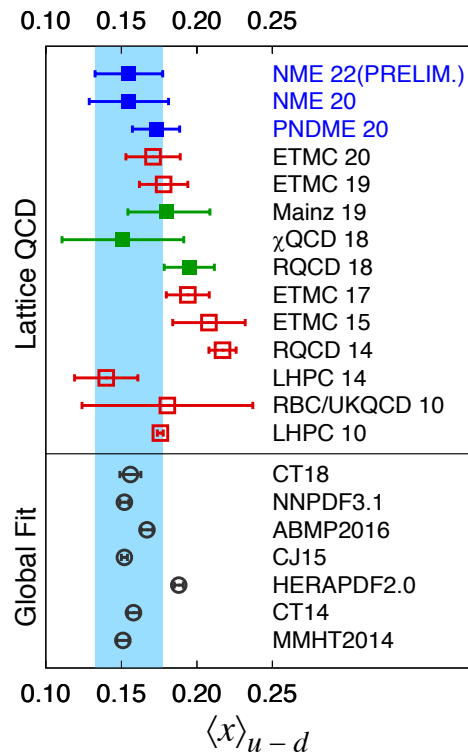
Moments of quark distributions (EIC and JLab)

- Momentum fraction (spin independent, ie, unpolarized quarks)
 - $\langle x \rangle_q = \int_0^1 x [q(x) + \bar{q}(x)] dx$ where $q = q_\uparrow + q_\downarrow$
- Helicity moment: quark helicity [anti] aligned with a longitudinally polarized proton
 - $\langle x \rangle_{\Delta q} = \int_0^1 x [\Delta q(x) + \Delta \bar{q}(x)] dx$ where $\Delta q = q_\uparrow - q_\downarrow$
- Transversity moment: quarks spin [anti] aligned with a transversely polarized proton
 - $\langle x \rangle_{\delta q} = \int_0^1 x [\delta q(x) + \delta \bar{q}(x)] dx$ where $\delta q = q_\top + q_\perp$

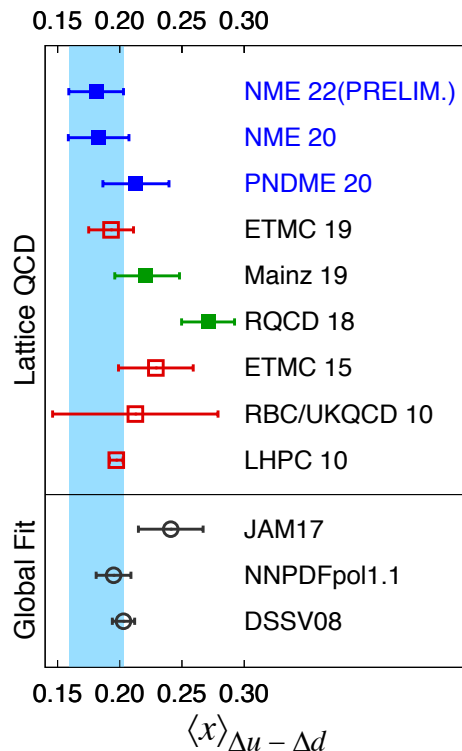
These first moments of twist two distribution functions are the first steps in the detailed tomography of the proton that will be explored at the EIC. Lattice QCD results are competitive



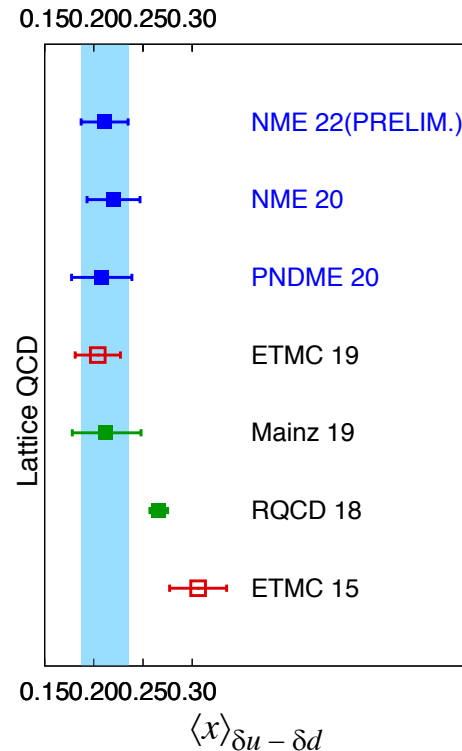
Moments of distributions



Momentum fraction



helicity moment



transversity moment



Conclusions: Impacts

- LANL results dominate FLAG global averages for Nucleon Matrix Elements
 - Axial charges (g_A , quark contribution to spin of the proton)
 - Scalar charges ($\sigma_{\pi N}$, strangeness content) (in FLAG 2023)
 - Tensor charges (transversity, quark contribution to nEDM)
- 3 new high impact results in 2021:
 - Axial vector form factors
 - nEDM from Θ -term
 - The pion-nucleon sigma term $\sigma_{\pi N}$ (direct detection of dark matter)



Future

- Results from 13 ensembles of 2+1-flavor clover ensembles
- Transition matrix elements: $\langle N \pi | O | N \rangle$, $\langle N N | O | N N \rangle$, ...
- Improve control over excited-state contamination for all nucleon matrix elements
- Methods to beat the signal-to-noise problem for all nucleon correlation functions
 - Normalizing flows for lattice generation
 - Contour deformation to deal with the signal-to-noise problem

