All about the Neutron from Lattice QCD

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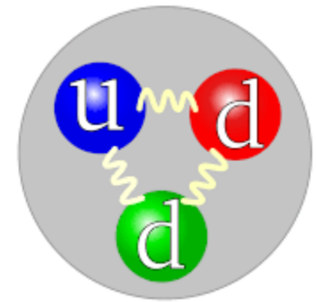
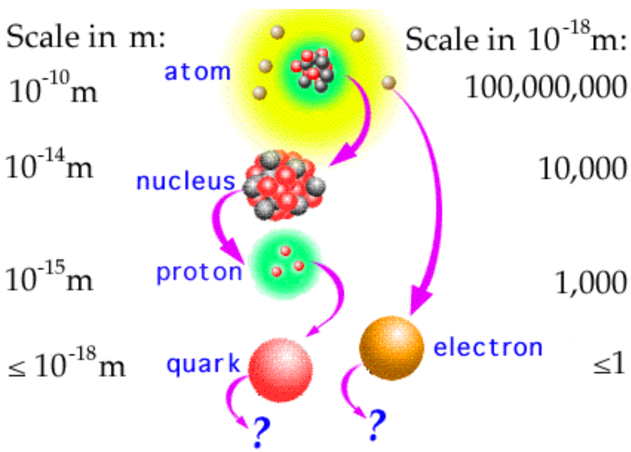
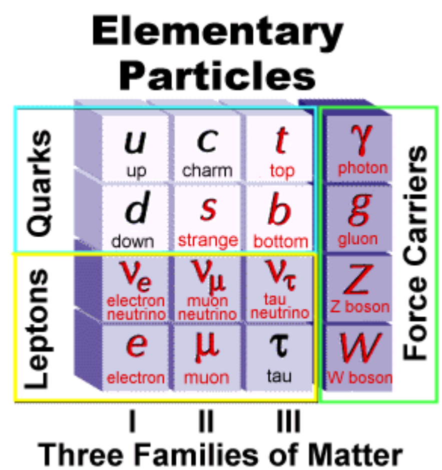
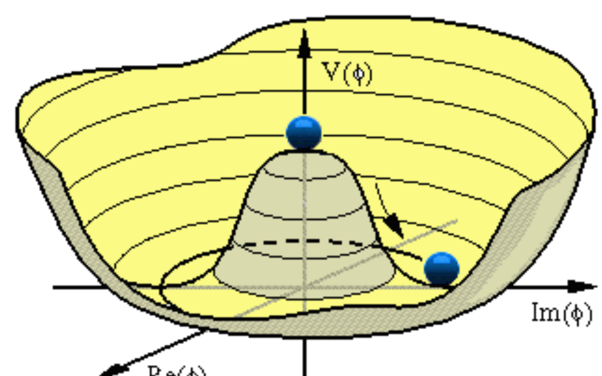








LA-UR: 16-29009, 17-23678, 18-25335, 19-25275

ISMD 2022, Pitlockry, 4 August 2022

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

PNDME and NME members

- 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 etal, 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

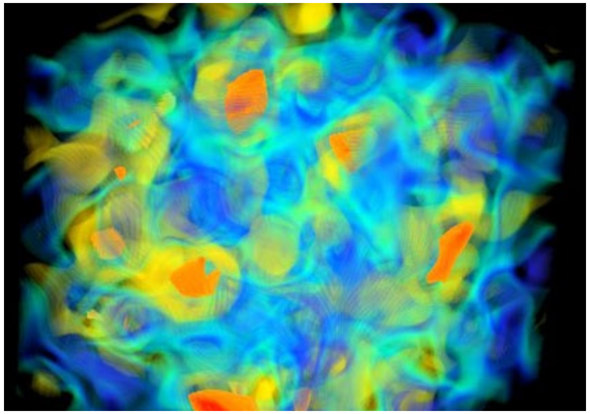
Lattice QCD is the best-known method for non-perturbative calculations of

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

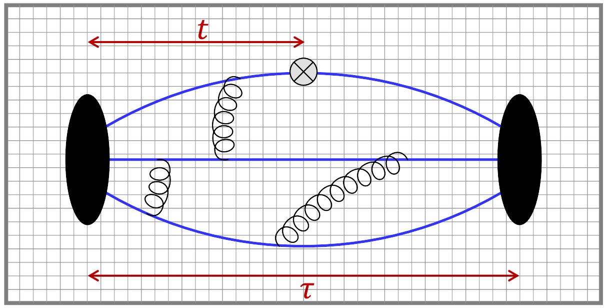
GOAL: Elucidate nucleon structure and decays using large scale simulations of lattice QCD.
Calculate the matrix elements of quark and gluon operators within the nucleon state.

LQCD is formulated as a Feynman path integral.

Simulations provide a stochastic computation of



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



What is the same in Minkowski and Euclidean Time?

- Time evolution: $e^{iHt} \rightarrow T \equiv e^{-H\tau}$
- Spectrum: $e^{iEt} \rightarrow e^{-E\tau}$ under $t \rightarrow i\tau$
- Matrix elements @ fixed time

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

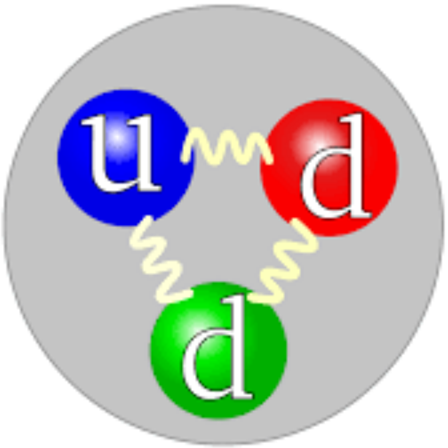
- Charges $g_A, g_S, g_T, \sigma_{\pi N}, \sigma_s$
- Axial & EM form factors
- Neutron electric dipole moment nEDM
- Neutrinoless double beta decay $0\nu\beta\beta$

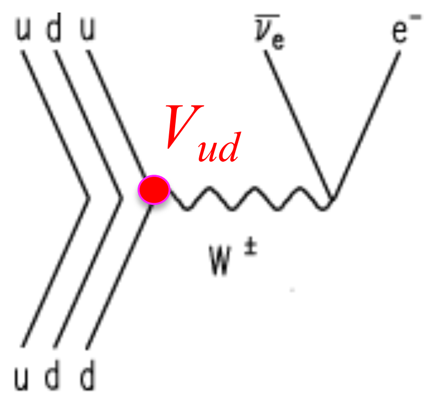
The neutron is a clean but challenging system

Decays weakly ⇒ a stable bound state of QCD

Properties:

- Charges g_A , g_P, g_S , g_T, g_V
- Spin content
  - Quarks
  - Gluons
- EDM
- Form factors
  - Electric, Magnetic
  - Axial
- Distribution functions, moments
  - PDF
  - GPD
- Radiative Corrections to decay





Numerical simulations of lattice QCD

- QCD on a 4D Euclidean grid with lattice spacing a
- Input Parameters: $\{a \leftrightarrow coupling, m_l \leftrightarrow M_\pi, m_s, m_c\}$
- Derivatives → finite differences
  - Discretization errors ($a \to 0$)
  - $O(a)$ improved actions
- Finite volume ($M_\pi L \to \infty$)
  - FV errors exponentially small for $M_\pi L > 4$
- Chiral extrapolation ($M_\pi \to 135$ MeV)
- Numerical integration of the path integral
  - Statistical errors
- Chiral symmetry plays an important role

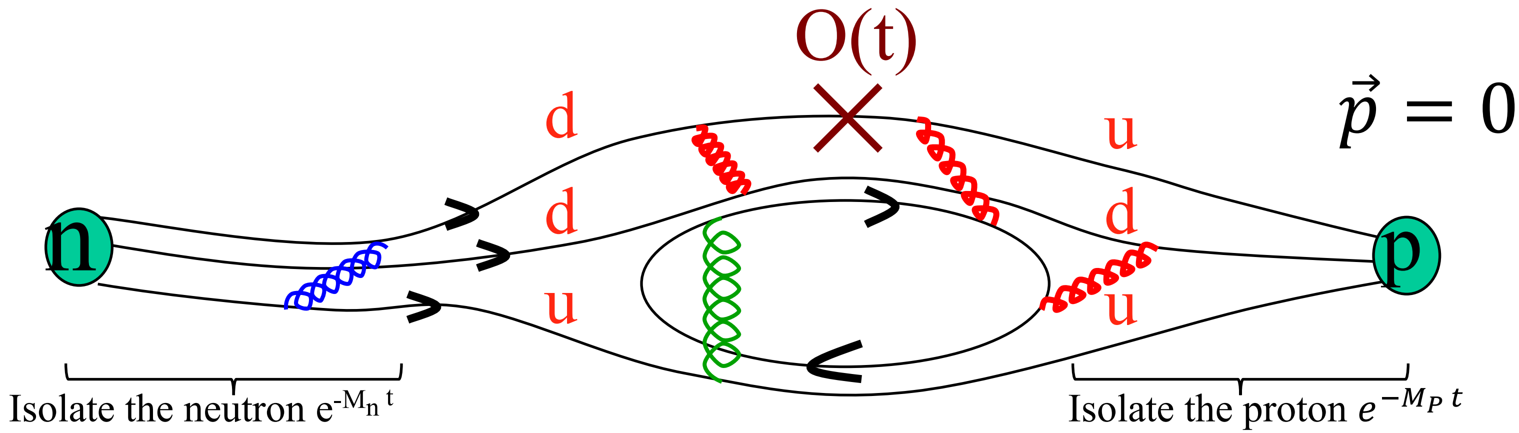
LQCD Methodology

- Generate gauge configurations (provide the quantum vacuum stochastically)
- Formulate operators that best probe the physics
  - Low energy effective operators encapsulating SM & BSM physics
  - Examples: Axial, scalar, tensor and vector quark bilinears ($O = \overline{q_\alpha} \, \Gamma_i \, q_\beta$), …
- Calculate quark propagators $S_F = \frac{1}{D}$ on the gauge configurations
- Construct hadronic correlation functions by tying S_F and gauge links
- Isolate ground state (→ "stochastic" quantum wavefunctions $|N(p_i)\rangle$)
- Calculate matrix elements: $\langle N(p_f) | O\ (Q^2) | N(p_i) \rangle$

Symmetries

- Gauge invariance
- Momentum conservation, not energy
- C, P, T
- "Chiral symmetry"

At finite t and τ, use the spectral decomposition of 2- and 3-point functions to remove ESC



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

$$\Gamma^3(t,\Delta t) = |A_0|^2 \langle 0|O|0\rangle e^{-M_0 \Delta t} + |A_1|^2 \langle 1|O|1\rangle e^{-M_1 \Delta t} + A_0 A_1^* \langle 0|O|1\rangle e^{-M_0 \Delta t} e^{-\Delta M(\Delta t - t)} + A_0^* A_1 \langle 1|O|0\rangle e^{-\Delta M t} e^{-M_0 \Delta t} + ...$$

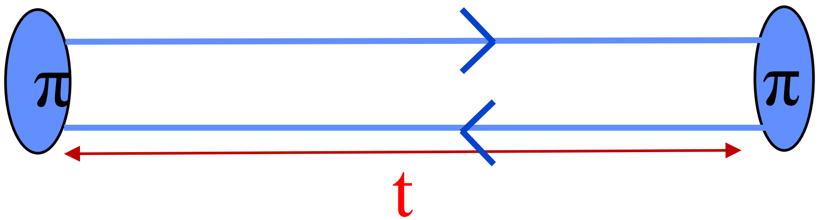
n-state fits to extract amplitudes, energy levels, matrix elements

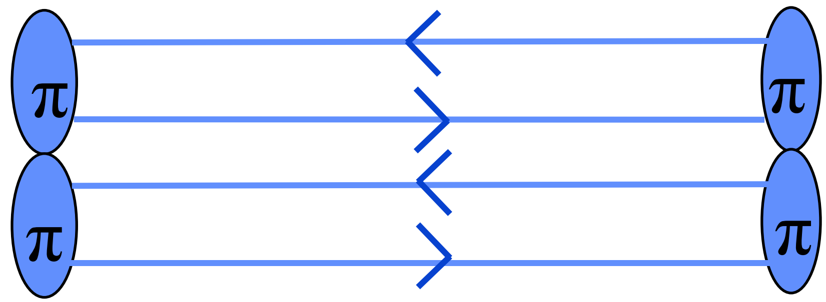
Challenge: Signal/Noise and excited state contamination in nucleon correlation functions

- Signal in all nucleon correlators degrades exponentially $\sim e^{-(M_N - 1.5 M_\pi)t}$

- Towers of low-mass excited states
  - $N_p \pi_{-p}$
  - $N_0 \pi_0 \, \pi_0$, $N_p (\pi\pi)_{-p}$, $N_0 \boldsymbol{\pi_p} \boldsymbol{\pi_{-p}}$, …

Signal-to-noise in pion's 2-point function Γ^2

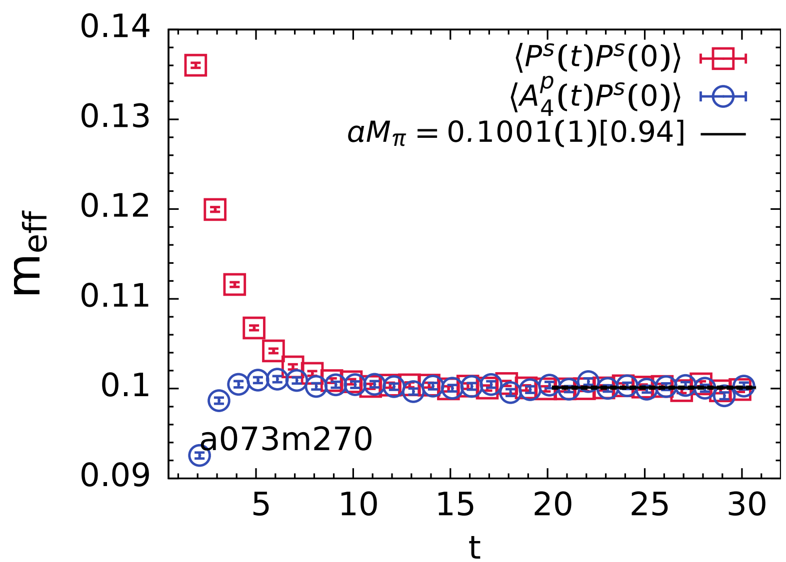




Signal: $\Gamma^2 \sim \; e^{-E_\pi t}$

Variance: $e^{-2E_\pi t}$

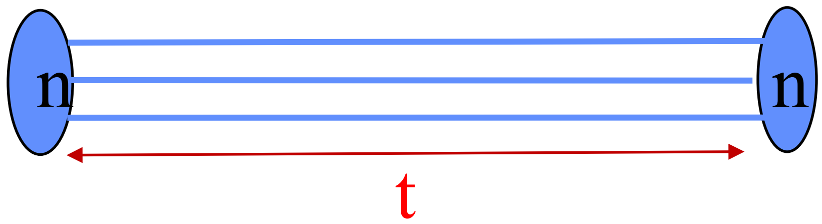
$$\Gamma^2(t) = |A_0|^2 e^{-M_0 t} + |A_1|^2 e^{-M_1 t} + |A_2|^2 e^{-M_2 t} + |A_3|^2 e^{-M_3 t} + \ldots.$$



$$M_{eff}(t) = \ln \frac{\Gamma^2(t)}{\Gamma^2(t+1)}$$

The signal does not degrade with t
The mass gap is large

Nucleon spectrum from 2-point function $\Gamma^2(t) = \langle\Omega|\overline{N}\,\mathrm{N}|\Omega\rangle$



$$\hat{N} = \epsilon^{abc}\left[q_1^{aT}(x)C\gamma_5\frac{(1\pm\gamma_4)}{2}q_2^b(x)\right]q_1^c(x)$$

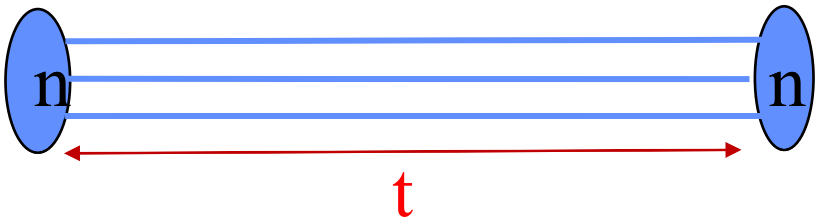
Spectral decomposition is same as for the pion

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

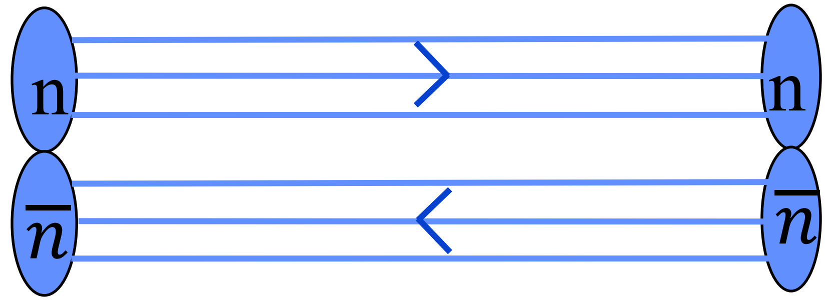
Fit the data for $\Gamma^2(t)$ versus t to extract

M_0, M_1, … masses of the ground & excited states
A_0, A_1, … corresponding amplitudes for creating/annihilating states

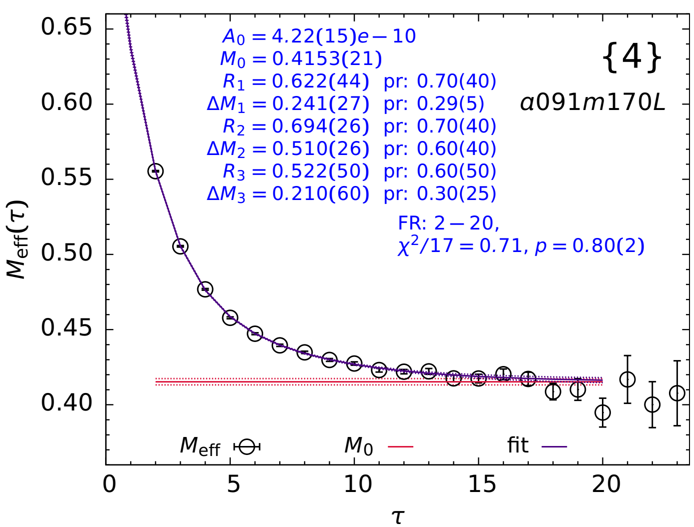
Signal-to-noise in the nucleon 2-point function Γ^2



Signal: $\Gamma^2 = e^{-E_N t}$



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

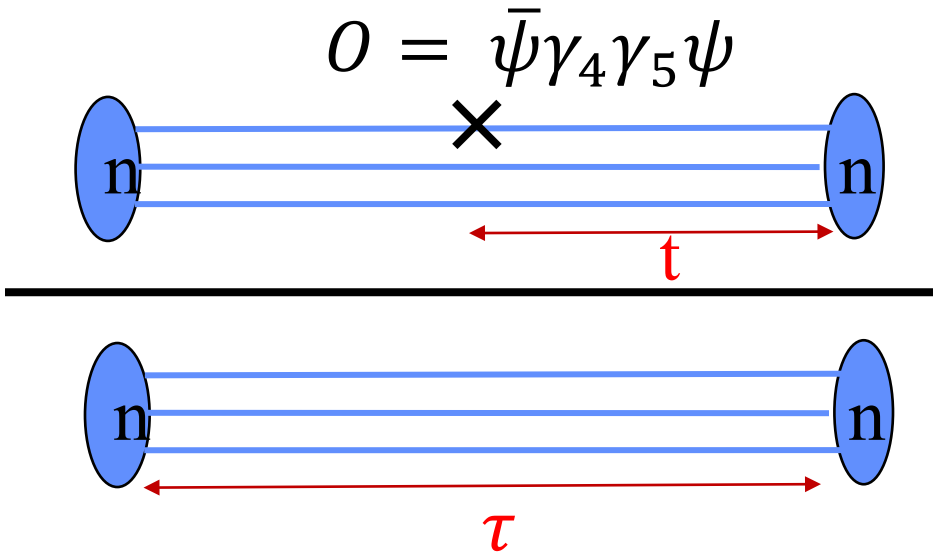


$$M_{eff}(t) = \ln \frac{\Gamma^2(t)}{\Gamma^2(t+1)}$$

- The signal/noise degrades exponentially $e^{-(M_N - 1.5M_\pi)t}$
- To resolve a <u>*small*</u> mass gap *($M_1 - M_0$) requires* large *t*

Calculating Nucleon Charges

$$\frac{\Gamma^3}{\Gamma^2} =$$



$$\rightarrow \boldsymbol{g_A}$$

$$\frac{\Gamma^3}{\Gamma^2} = \frac{\langle\Omega|\overline{N}\ A_\mu\ N|\Omega\rangle}{\langle\Omega|\overline{N}\ N|\Omega\rangle} \rightarrow \langle N(p_f)\big|A_\mu\ (Q^2)\big|N(p_i)\rangle \rightarrow \boldsymbol{g_A}$$

Excited states in correlation functions

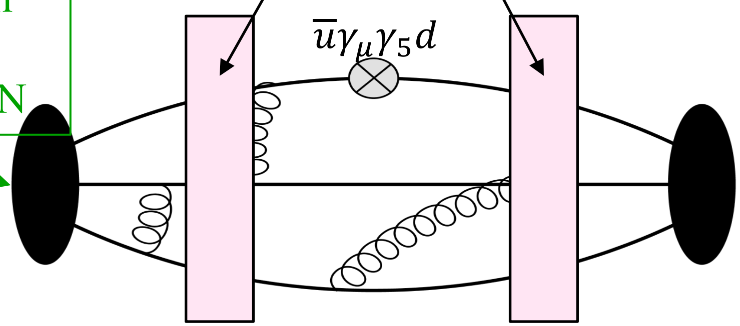
Challenge: To get the matrix elements within the nucleon ground state, the contributions of all excited states must be removed.

$$\hat{N} = \epsilon^{abc}\left[q_1^{aT}(x) C\gamma_5 \frac{(1 \pm \gamma_4)}{2} q_2^b(x)\right] q_1^c(x)$$

Interpolating operators create or annihilate all states with the same quantum numbers as N

Each intermediate state with nucleon quantum numbers is suppressed by the factor $\frac{A_i^2}{A_0^2} e^{-(M_i - M_N)t}$

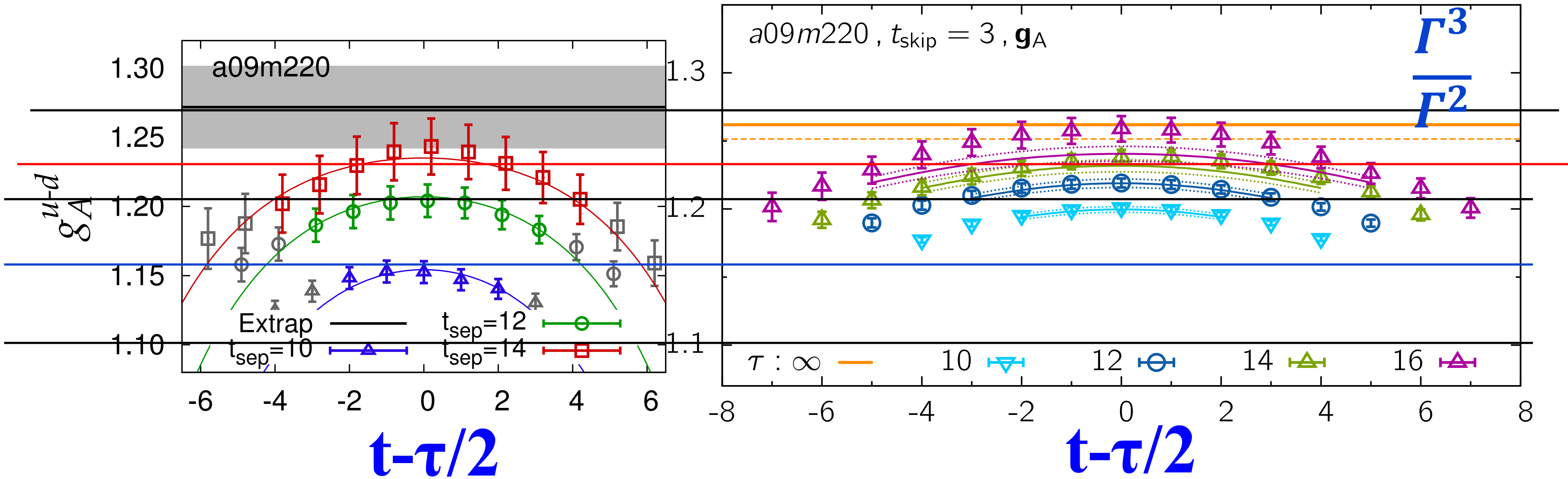
Towers of multihadron states
$N(\vec{p})\pi(-\vec{p})$
$N(0)\pi(\vec{p})\pi(-\vec{p})$
$N(\vec{p})2\pi(-\vec{p})$
…
+ radial excitations



- Which excited states make significant contributions to a given matrix element?
- What are their energies in a finite box?

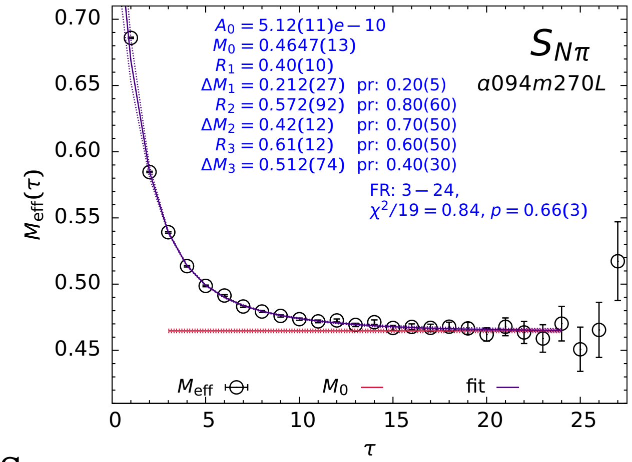
Fits to Γ^3 with ΔE_i from Γ^2 "work"

- Better smearing reduces ESC
- Higher statistics (10K➞500K) with bias corrected sloppy inversion method
- 4-5 values of source-sink separation τ
- 4-state fits to 2-point functions
- 3-state fits to 3-point functions
- Full covariance error matrix



Gupta et al, Phys. Rev. D98 (2018) 034503

Challenges for Nucleons



- Cannot go to large τ because the signal/noise degrades as $e^{-(M_N - 1.5 M_\pi)\tau}$
  - 2-pt: τ~ 2fm ; 3-pt: τ~1.5fm
- $\widehat{N}$ couples to the nucleon, all its excitations and multi-hadron states with the same quantum numbers
- As $\vec{q} \rightarrow 0$, the tower of $N\pi$, $N\pi\pi$ states becomes arbitrarily dense starting at ~1210 MeV
- The excited states that give significant contribution to a given ME are not known *a priori.*
- Large region in $\{E_i\}$ from 4-state fits to $\Gamma^2(t)$ have similar χ^2
- χPT is a good guide

Results from lattice QCD

The QCD community publishes, every two years, the review Flavor Lattice Averaging Group (FLAG) report
http://flag.unibe.ch/2021/

FLAG 2019: arXiv:1902.08191
FLAG 2021: arXiv:2111.09849

So far, the Nucleon Matrix Elements (NME) reviewed are

- Isovector charges g_A^{u-d}, g_T^{u-d}, and g_S^{u-d}
- Flavor diagonal charges: $g_A^{u,d,s,c}$, $g_S^{u,d,s,c}$, and $g_T^{u,d,s,c}$

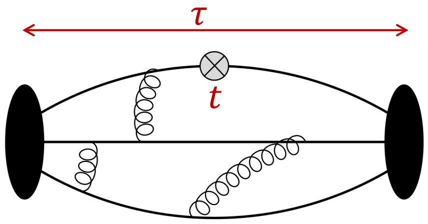
Lattice Methodology is well established

Isovector Nucleon Charges

Nucleon charges g_A^{u-d}, g_S^{u-d}, and g_T^{u-d} obtained from ME of local quark bilinear operators $\bar{q}_i\,\Gamma\,q_j$ within ground state nucleons:

$\langle N|\bar{q}_i\,\Gamma_O\,\tau^3\,q_j|N\rangle \propto g_O^{u-d}$

Connected diagram



Isovector Charges: probed in weak decays

g_A^{u-d}: axial charge (2-3%)
g_S^{u-d}: scalar charge (~10%)
g_T^{u-d}: tensor charge (~5%)

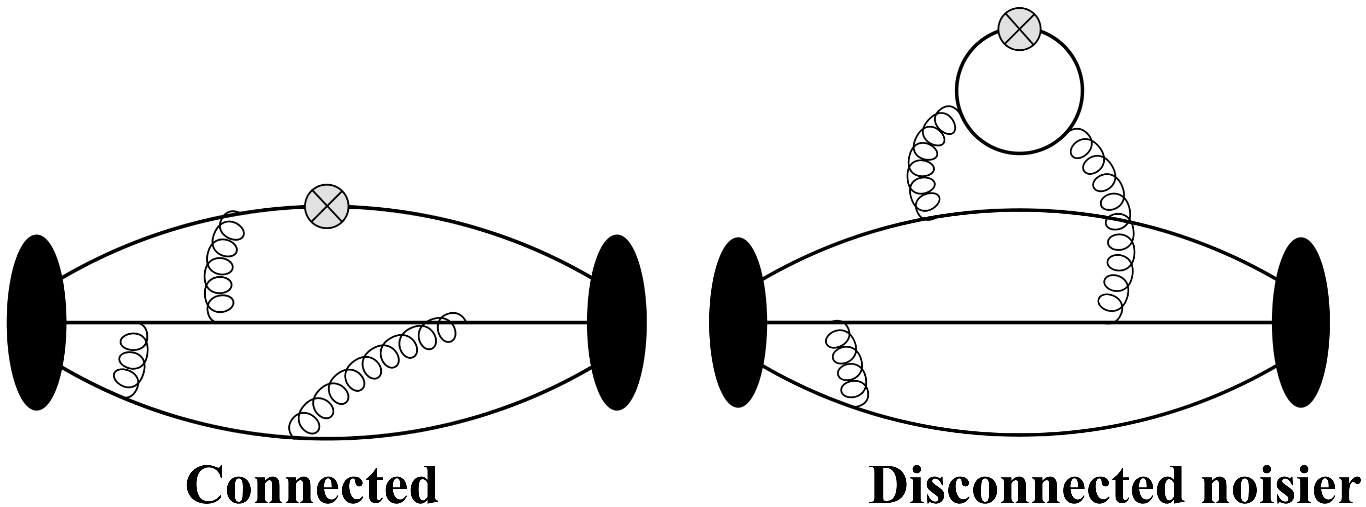
} Neutron beta decay

g_S^{u-d} and g_T^{u-d} combined with neutron decay parameters *b, B* probe novel scalar and tensor interactions at the TeV scale

PhysRevD.85.054512

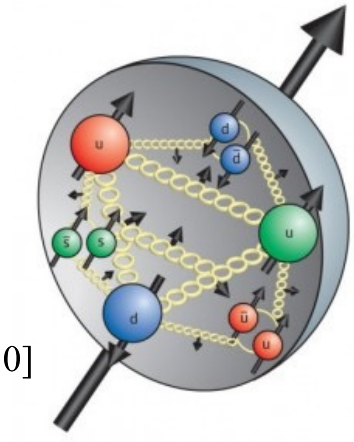
Flavor diagonal charges

$g_A^{u,d,s,c}$: Contribution of quark spin to nucleon spin
$g_S^{u,d,s,c}$: pion-nucleon sigma term, strangeness and charm content
$g_T^{u,d,s,c}$: Contribution of quark EDM to nucleon EDM, transversity



$$g_{A,S,T}^{u+d} = g_{A,S,T}^{u+d,\text{conn}} + 2g_{A,S,T}^{l,disc}$$

quark contribution to proton spin: $g_A^{u,d,s,c}$



gauge invariant decomposition of the proton spin is given by

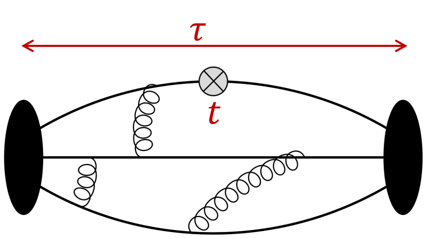
$$\frac{1}{2} = \sum_{\{u,d,s,c\}} \left(\frac{1}{2}\Delta q + L_q\right) + J_g$$

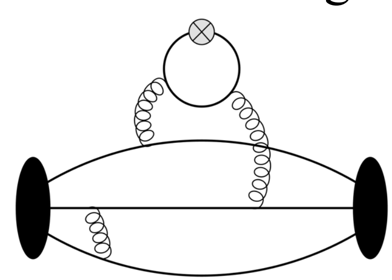
[X. Ji, PRL 78 (1997) 610]

$$S_P^q = \sum_q S_q \equiv \sum_q \frac{\Delta q}{2} \equiv 0.5 \sum_q g_A^q$$

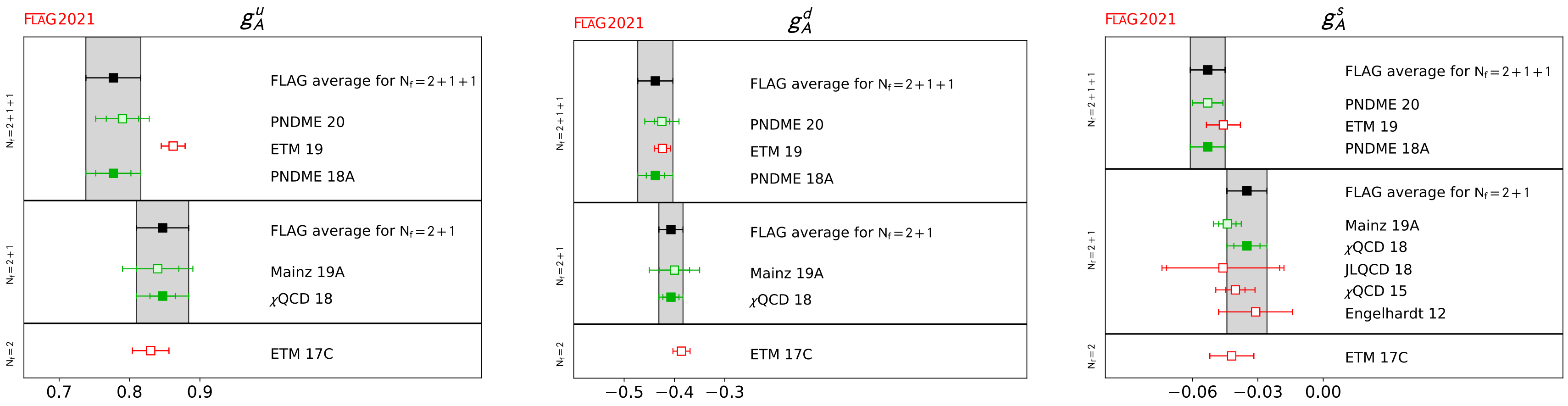
$$g_A^q = \langle N(p_i) | Z_A A_\mu^q(0) | N(p_i) \rangle$$

connected + disconnected diagrams





Spin of the proton



LANL (PNDME) result (PRD 98 (2018) 094512):

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

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

The pion-nucleon sigma term

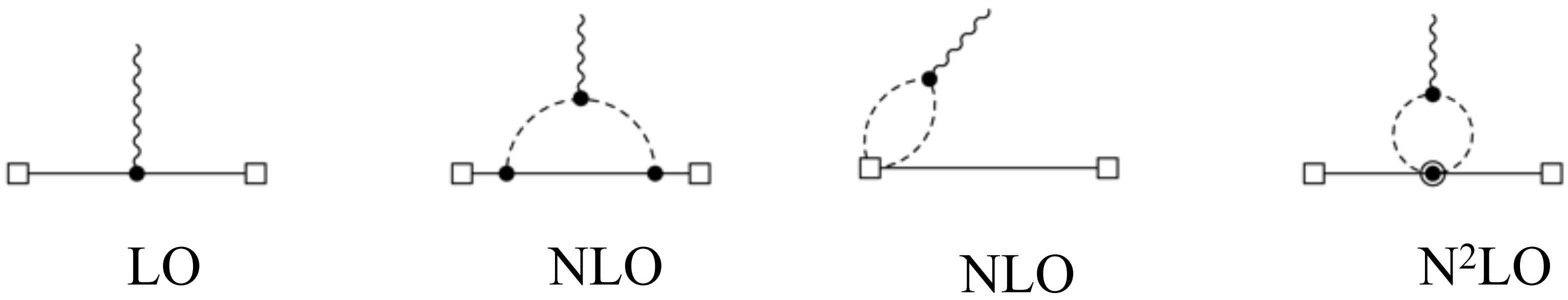
$$\sigma_{\pi N} \equiv m_{ud} g_S^{u+d} \equiv m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle$$

- 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

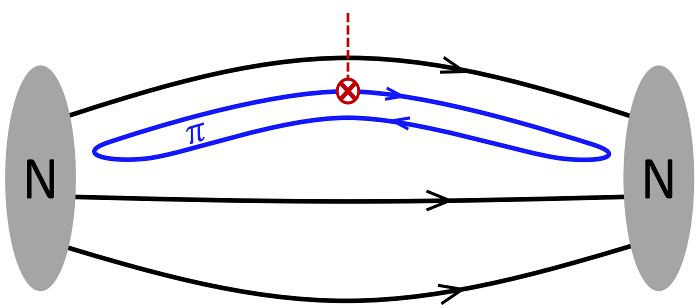
PRL 127 (2021) 242002; e-Print: 2105.12095
Rajan Gupta, Sungwoo Park, Martin Hoferichter, Emanuele Mereghetti, Boram Yoon, Tanmoy Bhattacharya

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

Coupling of S to $\pi\pi$ is large

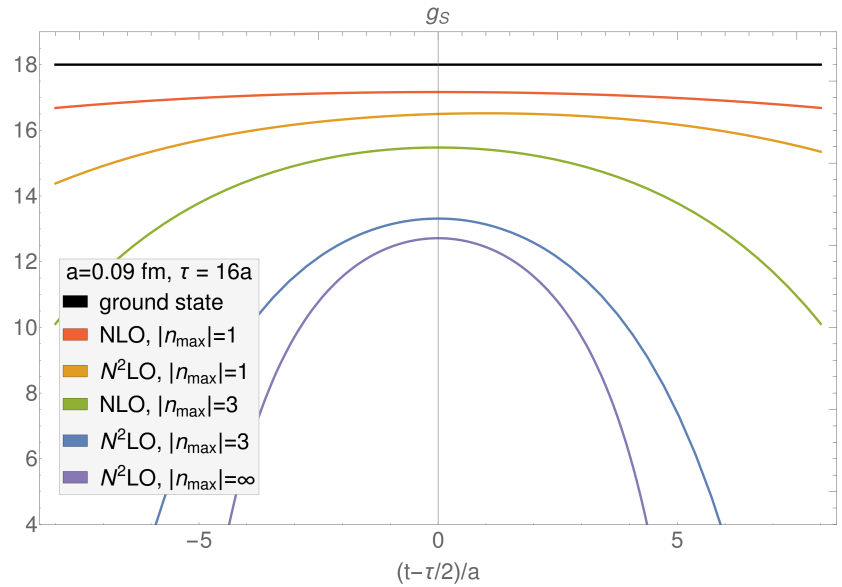


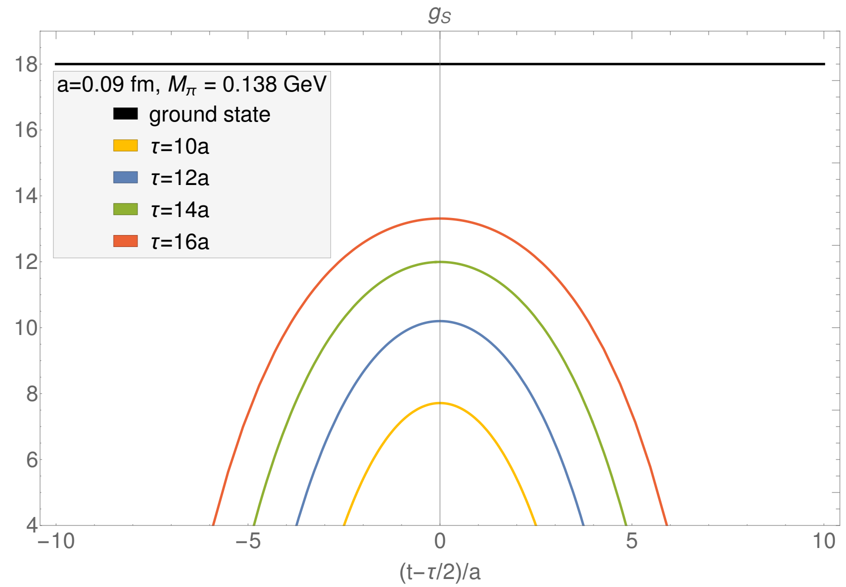
Why disconnected contribution is large



PRL 127 (2021) 242002

g_S: ESC from $N\pi$ & $N\pi\pi$ in N²LO χPT





Different truncations (χPT order and $\vec{p}$)

N²LO χPT estimates for $\tau = 10,12,14,16$

Estimates for the $a \approx 0.09 fm$; $M_\pi \approx 135 MeV$ ensemble assuming the asymptotic value is 18

The NLO and N²LO ESC can each reduce $\sigma_{\pi N}$ at a level of 10 MeV

Including the Δ as an explicit degree of freedom does not change the conclusions

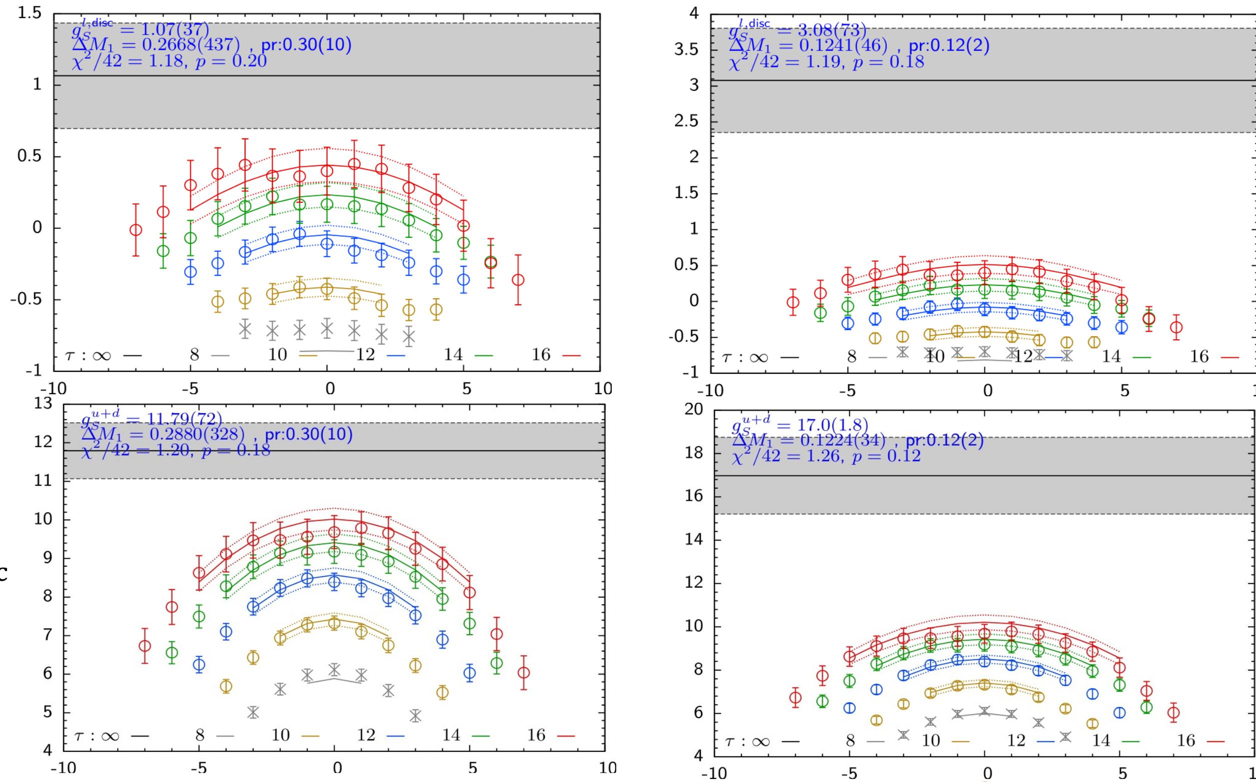
• e-Print: 2105.12095 [hep-lat]

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

Fits without $N\pi/N\pi\pi$ $(M_1 \approx 1.6\ GeV)$ with $N\pi$ / $N\pi\pi$ $(M_1 \approx 1.2\ GeV)$

$g_S^{l,\mathrm{disc}}$

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



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

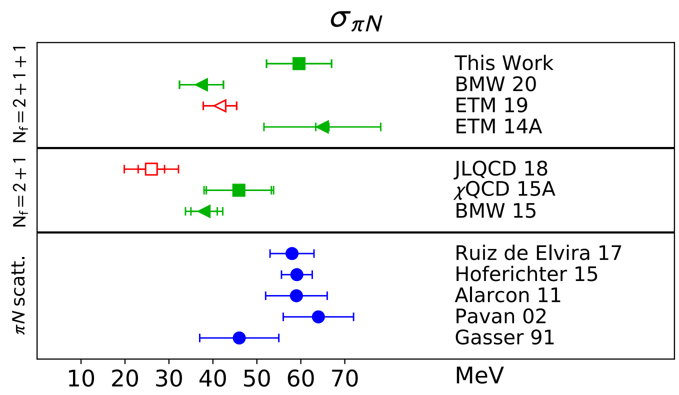
$\sigma_{\pi N} = m_l g_S^{u+d} \sim 60$ MeV

PRL 127 (2021) 242002

Resolved Tension Between Lattice QCD and Phenomenology

FLAG Reports 2019, 2021:

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



Post FLAG 2021 results

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

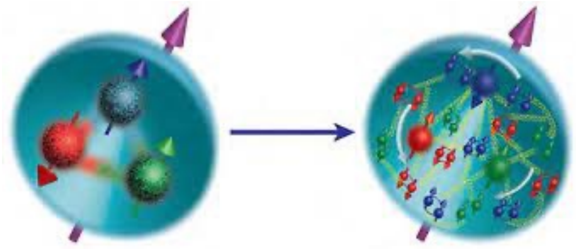
ETM (PRD **102**, 054517) $\sigma_{\pi N}$ = 41.6(3.8) MeV (Direct)

LANL Results: PRL 127 (2021) 242002; e-Print: 2105.12095

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

Moments of distributions

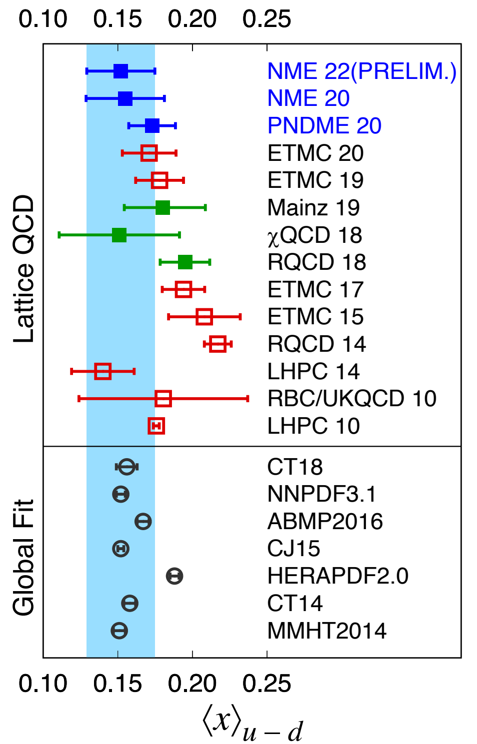
Moments of quark distributions (EIC and JLab)



- 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 $\delta q = q_\top + q_\perp$

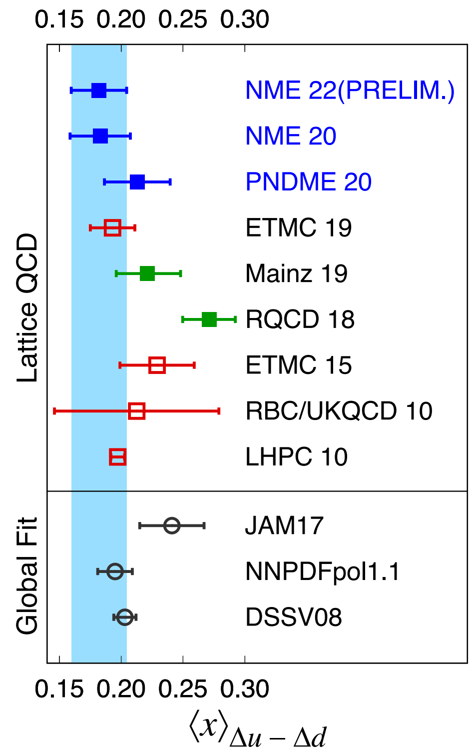
These first moments of twist two distribution functions are the first steps in the detailed 3-D tomography of the proton that will be explored at the EIC.
Lattice QCD results are competitive with global fits

Moments of distributions



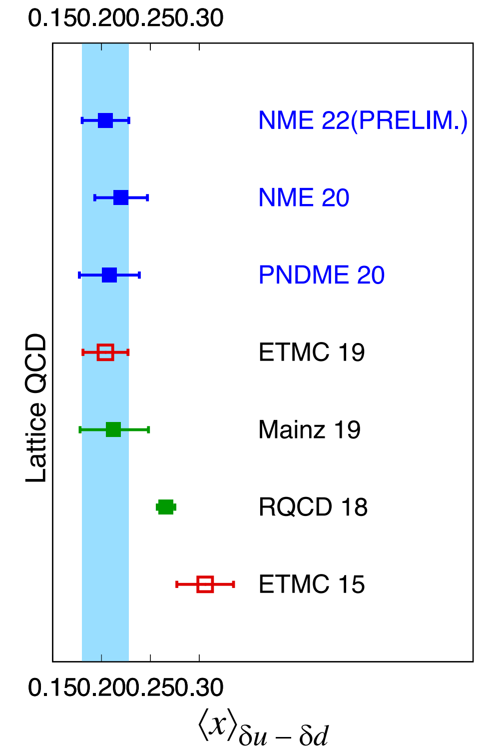
Momentum fraction

$$\langle x \rangle_q = 0.152(23)$$



Helicity moment

$$\langle x \rangle_{\Delta q} = 0.182(22)$$



Transversity moment

$$\langle x \rangle_{\delta q} = 0.204(24)$$

Error now dominated by ES uncertainty

LANL results: PRD 102 (2020) 054512; JHEP 04 (2021) 044, unpublished

Lattice QCD is providing many results with fully controlled errors that are testing the standard model and probing BSM physics