Excited States in Nucleon Matrix Elements

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

PNDME and NME members

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- Vincenzo Cirigliano (T-2 \rightarrow INT, UW)
- Rajan Gupta (T-2)
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- Boram Yoon (CCS-7)
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- 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:
- AFF:
- AFF:
- VFF:
- $\sigma_{\pi N}$
- d_n from Θ -term
- d_n from qEDM
- Moments of PDFs
- Proton spin:

NME

- Charges, FF:
- Moments of PDFs

- Gupta et al, PRD.98 (2018) 034503 Gupta et al, PRD 96 (2017) 114503 Jang et al, PRL 124 (2020) 072002 Jang et al, PRD 100 (2020) 014507 Gupta et al, PRL 127 (2021) 242002 Bhattacharya etal, PRD 103 (2021) 114507 Gupta et al, PRD 98 (2018) 091501 Mondal et al, PRD 102 (2020) 054512 Lin et al, PRD 98 (2018) 094512
- Park et al, PRD 105 (2022) 054505 Mondal et al, JHEP 04 (2021) 044

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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.

Simulations of LQCD turn a Quantum Field Theory (QCD) into a stocastic computational problem. They provide

- The quantum vacuum of QCD
 - > ensembles of gauge configurations

Hadrons & interactions put in as external probes
 N-point correlation functions

• Quantum wavefunctions of hadronic states > Matrix elements: $\langle N(p_f) | O(Q^2) | N(p_i) \rangle$







LQCD Methodology

- Generate gauge configurations
- Calculate quark propagator $S_F = \frac{1}{D}$ and construct hadronic states
- Isolate ground state wavefunctions $|N(p_i)\rangle$
- Formulate operators that best probe the physics
 - Low energy effective operators encapsulating SM & BSM physics
 - Examples: Axial, scalar, tensor and vector quark bilinears ($O = \overline{q} \Gamma_i q$), ...
- Calculate matrix elements: $\langle N(p_f) | O(Q^2) | N(p_i) \rangle$



Ingredients and Challenges

- Generate gauge configurations
 - New ideas: normalizing flows (autocorrelations, topology,)
- Calculate quark propagator $S_F = \frac{1}{D}$ and construct hadron correlators
 - Multigrid is very efficient
- Statistics: signal in correlation functions
 - Signal to noise (S2N) for nucleons degrades exponentially $e^{-(M_N-1.5M_\pi)\tau}$
- Isolate ground state wavefunctions $|N(p_i)\rangle$
 - Need to control large excited state contamination in all NME
- Formulate operators that best probe the physics
 - O(a) Improvement, Renormalization, Mixing
- Calculate matrix elements: $\langle N(p_f) | O(Q^2) | N(p_i) \rangle$
 - Contractions (improved operators, variational, multihadron states) expensive

Rich Landscape of LQCD calculations



The neutron is a clean but challenging system

Decays weakly \Rightarrow 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





Physics from nucleon matrix elements

- Isovector charges g_A, g_S, g_T
- Axial vector form factors
- Vector form factors
- Flavor diagonal matrix elements
- nEDM: Θ-term, quark EDM, quark chromo EDM, Weinberg operator, 4-quark operators
- 0νββ
- Generalized Parton Distribution Functions
- Radiative corrections to neutron decay

 $\begin{array}{l} \left\langle p | \overline{u} \Gamma d | n \right\rangle \\ \left\langle p(q) | \overline{u} \gamma_{\mu} \gamma_{5} d(q) | n(0) \right\rangle \\ \left\langle p(q) | \overline{u} \gamma_{\mu} d(q) | n(0) \right\rangle \\ \left\langle p | \overline{q} q | p \right\rangle \end{array}$

Lattice Methodology well established for "connected" and "disconnected" 3-point correlation functions

disconnected contributions are noisier (stochastic method) for the same computational cost and smaller in value



Challenges for Nucleons

- S2N in all nucleon correlations degrades as $e^{-(M_N - 1.5M_\pi)\tau}$ Current extent of the signal
 - 2-pt: $\tau \sim 2 fm$

- 3-pt: τ~1.5fm



- \hat{N} couples to the nucleon, all its excitations and multi-hadron states $N\pi$, $N\pi\pi$, ... with the same quantum numbers
- As $\vec{q} \rightarrow 0$, the tower of physical $N\pi$, $N\pi\pi$, ... states becomes arbitrarily dense starting at ~1210 MeV
- The excited states that give significant contributions to a given ME are not known *a priori*

Signal-to-noise (S2N) in pion's 2-point function



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





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

S2N is a constant, ie, it does not degrade with *t*

The mass gap is large

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



Spectral decomposition has same form as for the pion

$$\Gamma^{2}(t) = |A_{0}|^{2} e^{-M_{0}t} + |A_{1}|^{2} e^{-M_{1}t} + |A_{2}|^{2} e^{-M_{2}t} + |A_{3}|^{2} e^{-M_{3}t} + \dots$$

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

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

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





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

- The S2N degrades exponentially $e^{-(M_N-1.5M_\pi)t}$
- To resolve a <u>small</u> mass gap $(M_1 M_0)$ requires large t

4-state fits for $\Gamma^2(\vec{p},t)$



4-state fits to 2-point function



Surprise: ΔM_1 consistent with $N\pi$

Large region of $E_{i>0}$ values give similar χ^2/dof

Excited states in correlation functions

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



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

Calculating Nucleon Charges

$$\Gamma^{2} = \sum_{i} A_{i}^{*} A_{i} e^{-E_{i}\tau} \qquad \Gamma^{3} = \sum_{i,j} A_{i}^{*} A_{j} \langle N_{i} | O | N_{j} \rangle e^{-E_{i}t} e^{-E_{j}(\tau-t)}$$





Fits to Γ^3 taking the ΔE_i from Γ^2 "work"

What is current industry standard

- Better smearing reduces ESC
- Higher statistics ($10K \rightarrow 100K$) with TSM
- 4-5 values of source-sink separations $\tau \preceq 1.5$ fm
- 4-state fits to 2-point functions, 3-state fits to 3-point functions
- Full covariance error matrix



Yoon et al, PRD 93 (2016) 114506; Gupta et al, PRD98 (2018) 034503

Homework: Which excited states contribute and how to determine their energies?

- \widehat{N} couples to all excited states with nucleon quantum numbers
 - $N_p \pi_{-p}$
 - $N_0 \pi_0 \pi_0$
 - _
 - *N(1410)*
- The spectrum of $N_p \pi_{-p}$, ... becomes dense as $p \to 0$
- What are energies of these multihadron states in a finite box?
 Only the ΔE_i are needed, not the A_i
- Which of these states contribute to a given ME?
- Fits to 2-point function give large ΔE_i (>N(1410))
- 4-state fits to $\Gamma^2(t)$ give a large region in E_i with similar χ^2
- 3-state fits to $\Gamma^3(t)$ with these E_i work (χ^2 reasonable)
- 3-state fits to $\Gamma^3(t)$ with $E_1 = E_{N\pi}$ work (χ^2 reasonable)

4 Examples: ESC in the determination of

- Axial vector form factors G_A , \tilde{G}_P , G_P
- The axial charge g_A
- Contribution of the Θ -term to the neutron EDM
- The pion-nucleon sigma term $\sigma_{\pi N}$

$$\Gamma^3 = \sum_{i,j} A_i^* A_j \langle N_i | O | N_j \rangle e^{-E_i t} e^{-E_j (\tau - t)}$$

Lepton-nucleon scattering



 $G_E(Q^2)$

 $G_M(Q^2)$

 $G_A(Q^2)$

 $\widetilde{G_P}(Q^2)$

The v-n differential cross-section:

GOAL: High precision results for axial, electric and magnetic form factors versus Q^2 needed for determining x-section of (ν , e, μ) scattering off nuclei

$$\begin{aligned} \frac{d\sigma}{dQ^2} \begin{pmatrix} \nu_l + n \to l^- + p \\ \bar{\nu}_l + p \to l^+ + n \end{pmatrix} \\ &= \frac{M^2 G_F^2 \cos^2 \theta_c}{8\pi E_\nu^2} \left\{ A(Q^2) \pm B(Q^2) \frac{(s-u)}{M^2} + C(Q^2) \frac{(s-u)^2}{M^4} \right\}, \end{aligned}$$

$$\begin{split} A(Q^2) &= \frac{(m^2 + Q^2)}{M^2} \left[(1 + \tau) F_A^2 - (1 - \tau) F_1^2 + \tau (1 - \tau) F_2^2 + 4\tau F_1 F_2 \\ &- \frac{m^2}{4M^2} \left((F_1 + F_2)^2 + (F_A + 2F_P)^2 - 4 \left(1 + \frac{Q^2}{4M^2} \right) F_P^2 \right) \right], \\ B(Q^2) &= \frac{Q^2}{M^2} F_A(F_1 + F_2), \\ C(Q^2) &= \frac{1}{4} (F_A^2 + F_1^2 + \tau F_2^2). \end{split} \qquad \begin{split} \hline F_A &= \text{axial form} \\ \tilde{F}_P &= \text{induced product} \\ \hline F_P &= \text{induced product}$$

 $\langle NA_{\mu}N \rangle \rightarrow$ linear combination of F_A , \tilde{F}_P $\langle NPN \rangle \rightarrow G_P$ $\langle NV_{\mu}N \rangle \rightarrow G_E$, G_M F_A = axial form factor \tilde{F}_P = induced pseudoscalar $G_E = F_1 - \tau F_2$ Electric $G_M = F_1 + F_2$ Magnetic $\tau = Q^2/4M^2$ $M = M_n = M_p \approx 939$ MeV $m = M_\pi$

Cohesive strategy for (e, μ , v)-Z scattering •5 Form Factors, g_A , μ , g_p^*

- $G_E(Q^2)$ Electric
- $G_M(Q^2)$ Magnetic
- $G_A(Q^2)$ Axial
- $\tilde{G}_P(Q^2)$ Induced pseudoscalar
- $G_P(Q^2)$ Pseudoscalar
- All 5 form factors are calculated together
- Precise experimental data exist for $G_E(Q^2)$ and $G_M(Q^2)$
- Axial ward identity relates $G_A(Q^2)$, $\tilde{G}_P(Q^2)$, $G_P(Q^2)$
- $G_E(Q^2 = 0) = 1$
- Conserved vector charge
- $G_M(Q^2 = 0) = \mu = 4.7058$ Magnetic moment
- $G_A(Q^2 = 0) = g_A = 1.277(2)$ Axial charge
- $\tilde{G}_P(Q^2 = 0.88m_\mu^2) = g_p^* = 8.06(55)$ Induced pseudoscalar charge

Axial-vector form factors



Calculate the 3 form factors on the lattice

- Axial: G_A
- Induced pseudoscalar: \tilde{G}_P
- Pseudoscalar: G_P

ground state matrix elements decomposed into G_A , \tilde{G}_P , G_P

$$\left\langle N(p_f) \Big| A^{\mu}(q) \Big| N(p_i) \right\rangle = \overline{u}(p_f) \left[\gamma^{\mu} G_A(q^2) + q_{\mu} \frac{\tilde{G}_P(q^2)}{2M} \right] \gamma_5 u(p_i)$$

$$\left\langle N(p_f) \Big| P(q) \Big| N(p_i) \right\rangle = \overline{u}(p_f) G_P(q^2) \gamma_5 u(p_i)$$

PCAC relation $\partial_{\mu}A_{\mu} = 2mP$ implies G_A , \tilde{G}_P , G_P must satisfy

$$2\hat{m}G_P(Q^2) = 2M_N G_A(Q^2) - \frac{Q^2}{2M_N}\tilde{G}_P(Q^2)$$

Pion pole-dominance (PPD) hypothesis states

$$\widetilde{G_P}(Q^2) = G_A(Q^2) \left[\frac{4M_N^2}{Q^2 + M_\pi^2} \right] \qquad \underbrace{\frac{\sqrt{2} q_\mu F_\pi}}_{\sqrt{2} g_{\pi NN} \gamma_5} A_\mu}_{\sqrt{2} q_\mu F_\pi}$$

If pion pole-dominance holds ⇒ there is only one independent form factor

Goldberger-Trieman relation at $Q^2 = 0$

$$F_{\pi} g_{\pi NN} = M_N g_A$$

2017: Showed axial form factors with E_i from Γ^2 violate PCAC Gupta et al, PRD 96 (2017) 114503

PCAC:
$$R_1 + R_2 = \frac{\hat{m} G_P}{M_N G_A} + \frac{Q^2 \tilde{G}_P}{4M_N^2} = 1$$

PCAC violated if one uses the spectrum from 2-point function



$N\pi$ state couples in the axial channel



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



2019: Resolution of PCAC and PPD

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, we showed PCAC and PPD are satisfied



$$\begin{array}{rcl} G_A \sim & 2 & --8 \ \% \\ \text{Impact} & \tilde{G}_P \sim & 25 & --35 \ \% \\ & G_P \sim & 25 & --35 \ \% \end{array}$$

Axial Form Factors (unpublished)



 $N\pi$ state needed to satisfy PCAC. Impact on \tilde{G}_P and \tilde{G}_P is large

- $G_A \sim 2-8\%$
- *G̃_P* ~ 25—35 % *G_P* ~ 25—35 %



Electric & Magnetic form factors

Matrix Elements of $V_{\mu} \rightarrow$ Dirac (F₁) and Pauli (F₂) form factors

$$\left\langle N(p_f) \left| V^{\mu}(q) \right| N(p_i) \right\rangle = \overline{u}(p_f) \left[\gamma^{\mu} F_1(q^2) + \sigma^{\mu\nu} q_{\nu} \frac{F_2(q^2)}{2M} \right] u(p_i)$$

Define Sachs Electric (G_E) and Magnetic (G_M) form factors $G_E(q^2) = F_1(q^2) - \frac{q^2}{4M^2}F_2(q^2), \qquad G_M(q^2) = F_1(q^2) + F_2(q^2)$

Electric & Magnetic FF with 12 ensembles



- 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 $\{a, m_{u,d}, M_{\pi}L\}$

PRD 105 (2022) 054505

The axial charge

 $g_A \equiv Z_A \langle P | \bar{u} \gamma_5 \gamma_3 d | N \rangle$

A fundamental low energy parameter of QCD that enters in the analysis of weak interactions of nucleons and nuclei



ESC in the extraction of axial charge



AFF $G_A(Q^2 \rightarrow 0)$ do not satisfy PCAC

AFF $G_A(Q^2 \rightarrow 0)$ with $N\pi$ satisfy PCAC

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: <u>2105.12095</u> Rajan Gupta, Sungwoo Park, Martin Hoferichter, Emanuele Mereghetti, Boram Yoon, Tanmoy Bhattacharya

χ PT 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



PRL 127 (2021) 242002

g_S : ESC from $N\pi$ / $N\pi\pi$ in N²LO χ PT



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: <u>2105.12095</u> [hep-lat]

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



PRL 127 (2021) 242002

The Feynman-Hellman method

$$\sigma_{\pi N} \equiv m_{ud} g_S^{u+d} \equiv \frac{m_{ud} \partial M_N}{\partial m} \equiv \frac{m \partial M_\pi^2}{\partial m} \frac{\partial M_N}{\partial M_\pi^2}$$

- Both M_N and $\sigma_{\pi N}$ have similar χ PT structure. The starting point is the χ PT expansion for M_N
- $N(\vec{k})\pi(-\vec{k}), N(0)\pi(\vec{k})\pi(-\vec{k}), \dots$ state contribution increases as $M_{\pi} \rightarrow 135$ MeV
- Any fit to M_N versus M_{π}^2 should be done using data in a range where the mass gap of these excited states is lower than N(1440)
- Our work suggest this is $M_{\pi} \leq 200 \text{ MeV}$



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

Contributions to Neutron Electric Dipole Moment (nEDM)

- $d_n = \sum_{O_i} \epsilon_i X_i$ 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
- 5 kinds of operators: Θ-term, qEDM, chromoEDM, Weinberg, 4-fermion
- Measure d_n and calculate X_i using LQCD \Rightarrow constrain ϵ_i (BSM models)

If $d_n \gtrsim 10^{-28} e \ cm \rightarrow CP$ 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 quark EDM to neutron EDM





Sungwoo Park at Lat2022

PRD 98 (2018) 091501

Contribution of the O-term to the neutron EDM

- $L_{\Theta} = \Theta \frac{i G^a_{\mu\nu} \tilde{G}^a_{\mu\nu}}{32\pi^2}$ 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 $d_n \le 1.8 \times 10^{-26}$ e cm) is unnaturally small
- Axion field proposed to explain this small coupling

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





Excited state effect can be large



- Value of X_{Θ} is small and the signal is poor
- χPT 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 π states!!

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

Outlook

- Statistics: Generating gauge configurations
 - New ideas: normalizing flows (autocorrelations, topology,)
- Signal in correlation functions
 - Signal to noise (S2N) for nucleons degrades exponentially $e^{-(M_N-1.5M_\pi)\tau}$
 - Contour deformation to remove noise from imaginary part
- Isolate ground state wavefunctions $|N(p_i)\rangle$
 - Variational method (GEVP)