Nucleon Charges from Lattice QCD

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In collaboration with
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A Virtual Tribute to Quark Confinement and the Hadron Spectrum 2021, Aug 2-6 July 2021, online
Lattice QCD

- Non-perturbative approach to solving QCD on discretized Euclidean space-time
  - Hypercubic lattice with lattice spacing $a$
  - Quark fields placed on sites
  - Gluon fields on the links between sites; $U_\mu$

- Numerical lattice QCD calculations using Monte Carlo methods
  - $t \rightarrow -i\tau$; $e^{-iHt} \rightarrow e^{-E\tau}$, $\int e^{iS} \rightarrow \int e^{-S_E}$
  - Computationally intensive
  - Use supercomputers

- Continuum results are obtained in $a \rightarrow 0$

- Has been successful for many QCD observables
  - Some results are with less than 1% error
Lattice QCD

• Correlation functions

\[ \langle O \rangle = Z^{-1} \int dU dq d\bar{q} \, O(U, q, \bar{q}) e^{-S_g} \overline{e}^{(D + m_q)q} \]

\[ = Z^{-1} \int dU \left[ O \left( U, (D + m_q)^{-1} \right) e^{-S_g} \det(D + m_q) \right] \]

• Monte-Carlo integration
  - Integration variable \( U \) is huge
    \[ N_s^3 \times N_t \times 4 \times 8 \sim 10^9 \]
  - Generate Markov chain of gauge configurations \( U \)
  - Calculate average as expectation value
    \[ \langle O \rangle \approx \frac{1}{N} \sum_i O_i \left( U, (D + m_q)^{-1} \right) \]
  - Calculation of \( O_i \left( U, (D + m_q)^{-1} \right) \): measurement
  - \( (D + m)^{-1} \) is computationally expensive
Physical Results from Unphysical Simulations

• Finite Lattice Spacing
  • Simulations at finite lattice spacings $0.6\text{ fm} \lesssim a \lesssim 0.15\text{ fm}$
  ⇒ Extrapolate to continuum limit, $a = 0$

• Heavy Pion Mass
  • Lattice simulation:
    Smaller quark mass → Larger computational cost and noisy results
  • Simulations at (heavy) pion masses $130\text{ MeV} \lesssim M_\pi \lesssim 310\text{ MeV}$
  ⇒ Extrapolate to physical pion mass, $M_\pi = M_\pi^{\text{phys}}$

• Finite Volume
  • Simulations at finite lattice volume: $M_\pi L = 3 \sim 6$
  ⇒ Extrapolate to infinite volume, $M_\pi L = \infty$
Nucleon Charges

- **Isovector charges:** \( g^{u-d}_{A,S,T} \)
  \[ \langle p | \bar{u} \Gamma d | n \rangle = g^{u-d}_\Gamma \bar{\psi}_p \Gamma \psi_n \]
  - In the isospin limit \((m_u = m_d)\),
    \[ \langle p | \bar{u} \Gamma d | n \rangle = \langle p | \bar{u} \Gamma u - \bar{d} \Gamma d | p \rangle = \langle n | \bar{d} \Gamma d - \bar{u} \Gamma u | n \rangle \]
  - Cancel contributions from disconnected diagrams
  - Less systematics; better precision

- **Flavor-diagonal charges:** \( g^{u}_{A,S,T}, g^{d}_{A,S,T}, g^{s}_{A,S,T}, ... \)
  \[ \langle p | \bar{q} \Gamma q | p \rangle = g^{q}_\Gamma \bar{\psi}_p \Gamma \psi_p \quad \text{for } q = u, d, s, ... \]
  - Need calculations of disconnected diagrams
  - More systematics; worse precision
Nucleon Isovector Charges

\[ \langle p | \bar{u} \Gamma d | n \rangle = g_{\Gamma}^{u-d} \bar{\psi}_p \Gamma \psi_n \]
Nucleon Isovector Charges

- **Axial charge** $g_A$
  - Weak interactions of nucleons
  - $g_A/g_V = 1.27641(45)(33)$ from cold neutron decay experiments (Märkisch, et al., PRL, 2019)
  - Nuclear beta decay, pion exchange between nucleons, nucleosynthesis, ...

- **Scalar and tensor charges** $g_S, g_T$
  - Helicity-flip parameters $b$ and $b'_v$ in neutron decay
    - $b = 0.34 g_S \varepsilon_S - 5.22 g_T \varepsilon_T$
    - $b'_v = 0.44 g_S \varepsilon_S - 4.85 g_T \varepsilon_T$
  - When combined with (ultra) cold neutron decay experiments, $g_S, g_T$ provides bounds on novel scalar and tensor interactions that can arise in BSM
    (Bhattacharya, et al., PRD 2012)
Extracting Nucleon Charges on the Lattice

$$\langle p | \bar{u} \Gamma d | n \rangle = g_{\Gamma}^{u-d} \bar{\psi}_p \Gamma \psi_n$$

- $g_{\Gamma}^{u-d}$ is extracted from the ratio of two- and three-point correlation functions
  $$\frac{C_{3pt}(t, \tau)}{C_{2pt}(\tau)} \rightarrow g_{\Gamma}^{u-d}$$
  - $C_{2pt}(\tau) = \langle 0 \mid \chi(\tau) \bar{\chi}(0) \mid 0 \rangle$
  - $C_{3pt}(t, \tau) = \langle 0 \mid \chi(\tau) O_{\Gamma}(t) \bar{\chi}(0) \mid 0 \rangle$
  - $\chi = \epsilon^{abc}[u^{aT} \gamma_5 (1 + \gamma_4) d^b] u^c$

- $\chi$ introduces excited states of nucleons
Removing Excited-state Contamination

• Excited-states (ES) effect exponentially diminishes for large Euclidean time
  • Separating proton sources far from each other leaves only the ground-state
  • But signal-to-noise ratio drops exponentially in time for baryons \( R \sim e^{-\left(M_N - \frac{3}{2}m_\pi \right)\tau} \)

• For reasonably small \( t \) and \( \tau \), fit correlators to a function including ES
  • \( C_{2pt}(\tau) = \sum_i |A_i|^2 e^{-M_i\tau} \)
  • \( C_{3pt}(\tau, t) = \sum_{i,j} A_i A_j^* \langle i | O_{\Gamma} | j \rangle e^{-M_i t - M_j (\tau - t)} \)
  • \( C_{3pt}(t, \tau) / C_{2pt}(\tau) \rightarrow g_{\Gamma}^{u-d} \text{ as } t \rightarrow \infty, (\tau - t) \rightarrow \infty \)

• Tower of possible excited states
  • Radial excitations: \( N(1440), N(1710), \ldots \)
  • Multi-hadron states: \( N(p)\pi(-p), N(0)\pi(0)\pi(0), \ldots \)
  • But, which states contribute significantly?
Removing Excited-state Contamination

• Excited state fits to $C_{2pt}$ gives large first ES mass $M_1 \gtrsim M_{N(1440)}$

• But various evidences advocate $M_1 \ll M_{N(1440)}$
  • PCAC relation between $G_A, \tilde{G}_P$, and $G_P$ is much better satisfied with smaller $M_1$
  • Nucleon $\sigma$-term results are consistent with $\chi$PT when $M_1 \sim M_{N\pi, N\pi\pi}$

PRL 124, 072002 (2020)
arXiv:2105.12095
Effect of $N\pi$ Excited States

- Excited state fit results with and without $N\pi$-state is huge:
  - Smaller $M_1 \to$ smaller mass gap $\Delta M_1 = M_1 - M_0 \to$ longer extrapolation in $t \to \infty, (\tau - t) \to \infty$ 
    \[ \left( C_{3pt}^\Gamma(t, \tau)/C_{2pt}(\tau) = g^{u-d}_\Gamma + O(e^{-\Delta M_1 t}, e^{-\Delta M_1 (\tau-t), e^{-\Delta M_1 \tau}}) \right) \]

- But $\chi^2$ of 3pt fits are not sensitive to the low-lying excited-state mass

- Larger effect with smaller pion mass

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Isovector Charges – Lattice Setup

### $N_f = 2 + 1$ Clover-on-Clover

<table>
<thead>
<tr>
<th>EnsID</th>
<th>$a$ (fm)</th>
<th>$M_\pi$ (MeV)</th>
<th>Volume</th>
<th>$M_\pi L$</th>
<th>Confs</th>
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<tbody>
<tr>
<td>a127m285</td>
<td>0.127(2)</td>
<td>285(5)</td>
<td>$32^3 \times 96$</td>
<td>5.87</td>
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<td>a094m270</td>
<td>0.094(1)</td>
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<tr>
<td>a094m270L</td>
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<td>269(3)</td>
<td>$48^3 \times 128$</td>
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<tr>
<td>a091m170</td>
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<td>170(2)</td>
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</table>

**arXiv:2103.05599**

### $N_f = 2 + 1$ Clover-on-HISQ

<table>
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<tr>
<th>EnsID</th>
<th>$a$ (fm)</th>
<th>$M_\pi$ (MeV)</th>
<th>Volume</th>
<th>$M_\pi L$</th>
<th>Confs</th>
</tr>
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<tbody>
<tr>
<td>a15m310</td>
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<td>a12m310</td>
<td>0.1207(11)</td>
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<td>a12m220S</td>
<td>0.1202(12)</td>
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<td>3.29</td>
<td>946</td>
</tr>
<tr>
<td>a12m220</td>
<td>0.1184(10)</td>
<td>227.9(1.9)</td>
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<td>4.38</td>
<td>744</td>
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<td>313.0(2.8)</td>
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<tr>
<td>a09m220</td>
<td>0.0872(07)</td>
<td>225.9(1.8)</td>
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<tr>
<td>a09m130</td>
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<td>135.6(1.4)</td>
<td>$96^3 \times 192$</td>
<td>3.7</td>
<td>675</td>
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**PRD 98, 034503 (2018)**
Chiral, Continuum, Finite volume Extrapolation

- CCFV fit ansatz

\[ g(a, M_\pi, M_\pi L) = c_1 + c_2 a + c_3 M_\pi^2 + c_4 \frac{M_\pi^2}{\sqrt{M_\pi L}} e^{-M_\pi L} \]

- Only axial charge shows small FV effect

- Final results of mean and statistical/systematic errors are obtained by averaging/comparing various excited state fit ansatzes and CCFV (CC) fits
Isovector Charges - Results

**Axial**

- **CVC**: Conserved vector current relation for $g_S$;  
  \[ g_S/g_V = (M_N - M_P)^{QCD}/(m_d - m_u)^{QCD} \]

- **Pheno.**: Extraction of $g_T$ from semi-inclusive deep-inelastic scattering (SIDIS) experimental data
Nucleon Flavor-diagonal Charges

\[ \langle p | \bar{q} \Gamma q | p \rangle = g^q_{\Gamma \psi} \Gamma \psi_p \]
Flavor-diagonal Axial Charge: $g_A^{u,d,s}$

- Proton spin decomposition

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

where $g_A^q \equiv \Delta q = \int_0^1 dx (\Delta q(x) + \Delta \bar{q}(x))$

- Need to calculate quark-line disconnected diagrams, in addition to connected ones, which is computationally expensive and noisy
Flavor-diagonal Axial charges - Current Status

- Only PNDME and $\chi$QCD’18 data are extrapolated to continuum limit
- Charm-quark results ($g_A^c$) can be found at
  - PNDME: Rui Zhang’s talk at Lattice 2021; ETMC: PRD 102, 054517 (2020)
Flavor-diagonal Tensor Charge: $g^u,d,s_T$

- Nonzero neutron electric dipole moment (nEDM) violates P and T, so CP \rightarrow nEDM is a sensitive probe of new sources of CP violation in BSM

- No nonvanishing nEDM has been observed, but next-generation experiments will reach $d_N \sim 10^{-28} e \cdot cm$, which is the magnitude of nEDM predicted by many models in BSM

- To constrain BSM models using experimental value (or bound) of $d_N$, one needs corresponding QCD matrix elements

- One of the leading effective CPV Lagrangian term is

  $$ \mathcal{L}^{qEDM}_{CPV} = -\frac{i}{2} \sum_{q=u,d,s,...} d_q \bar{q} \sigma_{\mu\nu} \gamma_5 q F^{\mu\nu} $$

- Neutron EDM from qEDM

  $$ d_N^{qEDM} = d_u g^u_T + d_d g^d_T + d_s g^s_T + \ldots $$
Flavor-diagonal Tensor charges - Current Status

<table>
<thead>
<tr>
<th></th>
<th>$g_T^u$</th>
<th>$g_T^d$</th>
<th>$g_T^s$</th>
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</thead>
<tbody>
<tr>
<td>PNDME ’18</td>
<td>0.784(28)(10)</td>
<td>-0.204(11)(10)</td>
<td>-0.0027(16)</td>
</tr>
<tr>
<td>ETMC ’20</td>
<td>0.729(22)</td>
<td>-0.208(8)</td>
<td>-0.0027(6)</td>
</tr>
</tbody>
</table>

- PNDME ’18 results are extrapolated to continuum limit from seven (six) ensembles for the strange (light) quarks: $M_\pi \approx 135, 220, 310$ MeV, $a \approx 0.06, 0.09, 0.12, 0.15$ fm
- ETMC ’20 results are from a single ensemble at $M_\pi = 139$ MeV, $a = 0.08$ fm
- Charm-quark results ($g_A^c$) can be found at
  - PNDME: Rui Zhang’s talk at Lattice 2021; ETMC: PRD 102, 054517 (2020)
BSM Constraints from Tensor Charge

• For models in which \( qEDM \) is the dominant BSM source of CP violation

\[
d_N = d_u g^u_T + d_d g^d_T + d_s g^s_T + \ldots
\]

• Known parameters

  • \( g^u_T = 0.784(28)(10), \ g^d_T = -0.204(11)(10), \ g^s_T = -0.0027(16) \)
  
• \( |d_N| < 1.8 \times 10^{-26} e \cdot cm \) [nEDM experiment, PRL. 124, 081803 (2020)]

⇒ Constraints on BSM couplings \( d_u, d_d, d_s \) (left), and allowed \( M_2 - \mu \) region for various values of \( d_n/d_e \) in split SUSY model (right)
Flavor-diagonal Scalar Charge: $g_S^{u,d,s}$

- Nucleon $\sigma$-terms

\[
\sigma_{\pi N} = m_{ud} \langle N | \bar{u}u + \bar{d}d | N \rangle = m_{ud} (g_S^u + g_S^d) \equiv g_S^{u+d}
\]

\[
\sigma_S = m_s \langle N | \bar{s}s | N \rangle = m_s g_S^s
\]

- Critical to include $N\pi$ excited-state (ES) terms to remove ES contamination

- Results with $N\pi$ ES-terms gives consistent chiral fit coefficients with $\chi$PT predictions

<table>
<thead>
<tr>
<th>chiral fit</th>
<th>$d_2$ (GeV$^{-1}$)</th>
<th>$d_3$ (GeV$^{-2}$)</th>
<th>$d_4$ (GeV$^{-3}$)</th>
<th>$d_{4L}$ (GeV$^{-3}$)</th>
<th>$\chi^2_{\text{dof}}$</th>
<th>$\sigma_{\pi N}$ (MeV)</th>
<th>$d_2$ (GeV$^{-1}$)</th>
<th>$d_3$ (GeV$^{-2}$)</th>
<th>$d_4$ (GeV$^{-3}$)</th>
<th>$d_{4L}$ (GeV$^{-3}$)</th>
<th>$\chi^2_{\text{dof}}$</th>
<th>$\sigma_{\pi N}$ (MeV)</th>
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<tr>
<td>$\chi$PT</td>
<td>4.44</td>
<td>-8.55</td>
<td>-</td>
<td>11.35</td>
<td>-</td>
<td>-</td>
<td>4.44</td>
<td>-8.55</td>
<td>-</td>
<td>11.35</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>${2,3}$</td>
<td>2.48(29)</td>
<td>-2.8(1.1)</td>
<td>-</td>
<td>-</td>
<td>0.68</td>
<td>38.3(2.8)</td>
<td>3.74(35)</td>
<td>-6.7(1.2)</td>
<td>-</td>
<td>47(25)</td>
<td>0.84</td>
<td>61.6(6.4)</td>
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<tr>
<td>${2,3,4}$</td>
<td>3.1(1.2)</td>
<td>-8(10)</td>
<td>10(20)</td>
<td>-</td>
<td>0.82</td>
<td>40.3(4.7)</td>
<td>6.7(1.6)</td>
<td>-31(13)</td>
<td>-</td>
<td>47(25)</td>
<td>0.84</td>
<td>61.6(6.4)</td>
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<tr>
<td>${2^x,3^x,4}$</td>
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<td>-4.07(71)</td>
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<td>12.2</td>
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<td>-0.5(11.7)</td>
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<td>5.57(96)</td>
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<td>45(23)</td>
<td>26(15)</td>
<td>0.77</td>
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<tr>
<td>${2,3^x,4,4L^x}$</td>
<td>3.86(17)</td>
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<td>11.35</td>
<td>0.87</td>
<td>44.5(2.4)</td>
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<td>1.41</td>
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<td>18.5(7.2)</td>
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<td>0.93</td>
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<tr>
<td>${2^x,3^x,4,4L^x}$</td>
<td>4.44</td>
<td>-8.55</td>
<td>22.51(71)</td>
<td>11.35</td>
<td>3.13</td>
<td>52.72(24)</td>
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<td>23.97(64)</td>
<td>11.35</td>
<td>0.86</td>
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arXiv:2105.12095
Current status of $\sigma_{\pi N}$ from Lattice QCD

- Phenomenological estimates using $\pi N$-scattering data gives $\sigma_{\pi N} \sim 60$ MeV
- Lattice results without $N\pi$ ES-terms gives $\sigma_{\pi N} \sim 40$ MeV
- Lattice result with $N\pi$ ES-terms gives $\sigma_{\pi N} = 61.6(6.4)$ MeV
Summary

• Nucleon charges play important role in analysis of experimental data and probing new physics in BSM

• Lattice QCD provides precise estimates of the nucleon charges

• Removing excited state contamination may need proper incorporation of $N\pi$ excited states

  • Current statistics does not provide a good determination of the first excited state, but indirect evidences (PCAC relation, $\chi$PT prediction) support strong effect of $N\pi$ excited states