Nucleon structure from lattice QCD

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The Cyprus Institute

CaSToRC

Outline

- **Introduction**
  - Hadron structure from the lattice
  - Computational issues: cost, simulations and analysis
- **Methods for hadron structure on the lattice**
  - Methods for excited state identification
- **Representative results**
  - Nucleon axial and tensor charge
  - Electromagnetic form factors of the nucleon
  - Nucleon σ-terms
  - Nucleon to Δ transition form factors
- **Outlook and summary**
  - Outlook on new methods for noise reduction
  - Summary

European Twisted Mass Collaboration

Lattice QCD

- **Post-diction of experimentally well known quantities**
  - Masses of low-lying hadrons
  - Nucleon axial-charge g_A
  - Nucleon momentum fraction $\langle x \rangle$
  - Nucleon electromagnetic form-factors

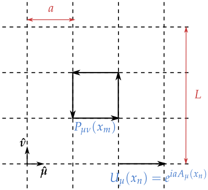
"Benchmark" or "Gold-plated" quantities

- **Pre-diction of experimentally less (or not) known quantities**
  - Nucleon scalar and tensor charges g_S, g_T
  - Nucleon sigma terms
  - Axial charges of hyperons
  - Neutron electric dipole moment
  - Precision measurements of proton radius, anomalous magnetic moment of muon (hadronic)

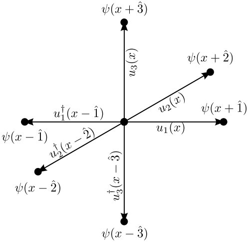
Contact to new physics

QCD on the lattice

4D space - time lattice



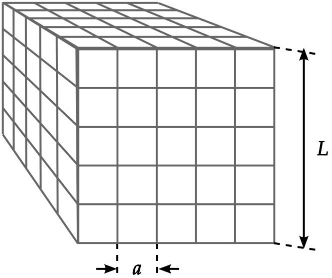
- 4D grid, spacing a, extent L
- Quark fields $\psi(x)$, $\bar{\psi}(x)$, gluon fields $U_\mu(x)$
- Finite $a \rightarrow$ UV cut-off
- Finite $L \rightarrow$ quantized momenta $\frac{2\pi}{L}\vec{n}$



- Monte Carlo simulation for ensembles of gluon fields, with probability $e^{S[U,M^{-1}]}$ (Euclidean time)
- Observables: $\langle O \rangle = \sum_{\{U\}} O(M^{-1}, U_\mu)$, with M^{-1} the quark propagator
- M, discrete covariant derivative (Dirac operator) $\rightarrow$ 4D stencil

- **Sources of uncertainty**
  - $\mathcal{O}$(1,000) to $\mathcal{O}$(100,000) independent statistics depending on observable and required precision
  - Take $a \rightarrow 0$ limit (3 lattice spacings)
  - Take $L \rightarrow \infty$ limit (2-3 volumes)
  - ~~M: ill-conditioned for $m_q \ll$, need several m_q to take $m_q \rightarrow m_q^{\text{phys}}$~~
    Simulations available at $m_q = m_q^{\text{phys}}$
  - Inclusion of disconnected quark loop contributions

- **Current state-of-the-art**
  - $L \gtrsim 5$ fm
  - $a \simeq 0.1$ fm
  - Lattice sizes $\gtrsim 48^3 \times 96 = \mathcal{O}(10^7)$ sites



Twisted mass fermions

Transform quark spinor fields $\psi = \binom{u}{d}$ to "Twisted Mass" basis:

$$\chi = \frac{1}{\sqrt{2}}(1 + i\gamma_5\tau_3)\psi, \quad \bar{\chi} = \frac{1}{\sqrt{2}}\bar{\psi}(1 + i\gamma_5\tau_3).$$

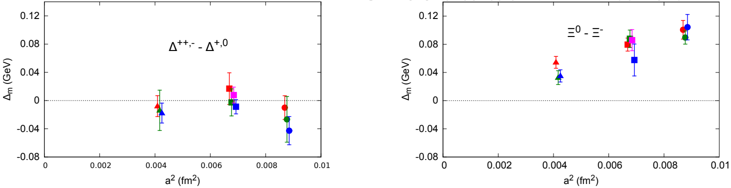
Twisted mass fermion action:

$$S_F = \bar{\chi} M \chi = a^4 \sum_x \bar{\chi}(x)[D[U] + m + i\mu\gamma_5\tau_3]\chi(x)$$

with $D[U] = \frac{1}{2}[\gamma_\mu(\nabla_\mu + \nabla^*_\mu) - a\nabla^*_\mu\nabla_\mu]$ the massless Wilson-Dirac operator

— $m = m_{\mathrm{crit}}$ "maximal twist":
- ✓ Automatic $O(a)$ improvement
- ✓ No additional operator improvement terms required
- ✗ Isospin breaking at $O(a^2)$

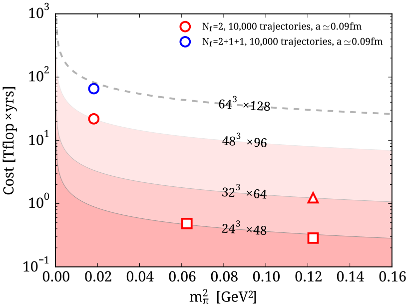
C. Alexandrou *et al.* `arXiv:1406.4310`



Small isospin breaking effects - worst case Ξ^0-Ξ^-

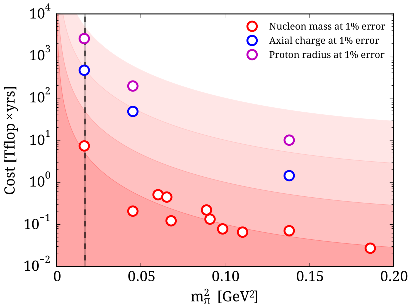
Simulation and analysis cost

Simulation cost



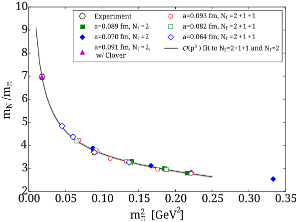
— Twisted mass fermions
— N_f=2 and N_f=2+1+1 flavors
— Empirical cost formula:
$C^{\text{sim}} \propto \left(\frac{0.3\text{GeV}}{m_{\text{PS}}}\right)^{C_m}\left(\frac{L}{2\text{fm}}\right)^{C_L}\left(\frac{0.1\text{fm}}{a}\right)^{C_a}$

Analysis cost

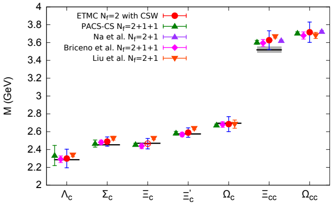


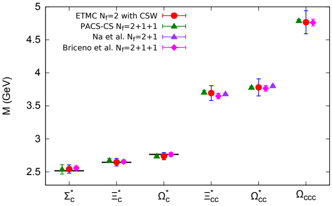
— Analysis cost dominated by inversion cost
— Up-scaled to $64^3 \times 128$
— Peta-flop sustained → Exa-flop requirements

Hadron masses



- Physical point simulation: agreement with physical m_N/m_π ratio
- Chiral fit to $m_\pi > m_\pi^{\text{phys}}$ lattice data reproduces the physical poin
- Agreement between $N_f = 2$ and $N_f = 2+1+1$ simulations

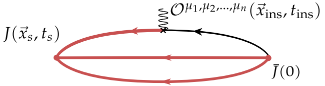




- Post-diction of observed charmed baryons (bands)
- Prediction of yet to be observed Ω_{cc}, Ω^*_{cc}, Ω_{ccc}, and Ξ^*_{cc}

C. Alexandrou *et al.* `arXiv:1411.3494`

Nucleon matrix element methods



- Matrix elements from three-point correlation functions

$$G_{3\rm pt}^{\mu_1,\ldots,\mu_n}(\Gamma_\nu, \mathbf{p}, \mathbf{q}, t_s, t_{\rm ins}) = \sum_{\mathbf{x}_s, \mathbf{x}_{\rm ins}} e^{-i\mathbf{x}_s\cdot\mathbf{p}} e^{-i\mathbf{x}_{\rm ins}\cdot\mathbf{q}} \Gamma^\nu_{\beta\alpha} \langle J_\alpha(t_s, \mathbf{x}_s) \mathcal{O}_\Gamma^{\mu_1,\ldots,\mu_n}(t_{\rm ins}, \mathbf{x}_{\rm ins}) \bar{J}_\beta(0)\rangle$$

- Form an appropriate ratio with two-point functions:

$$R(\Gamma^\lambda, t_s, t_{\rm ins}) \propto \mathcal{M} + \mathcal{R} e^{-\Delta(t_s - t_{\rm ins})} + \mathcal{R}^\dagger\, e^{-\Delta t_{\rm ins}} + O(e^{-\Delta' t_{\rm ins}})$$

- $\mathcal{M} = \langle N|\mathcal{O}|N\rangle$ desired matrix element
- Δ, Δ' energy gaps with 1st and 2nd excited states

a) Take large time extents to yield "plateau value"

$$R(\Gamma^\lambda, t_s, t_{\rm ins}) \xrightarrow[t_s - t_{\rm ins} \gg]{t_{\rm ins} \gg} \Pi(\Gamma^\lambda)$$

b) Sum over insertion time for "summation method"

$$\sum_{t_{\rm ins}} R(\Gamma^\lambda, t_s, t_{\rm ins}) = \text{Const.} + \mathcal{M} t_s + O(e^{-\Delta t_s})$$

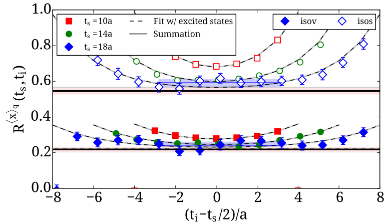
c) Fit including first excited state effects (Δ, $\mathcal{R}$)

Nucleon matrix element methods

Fit to plateau

✓ Fit to constant

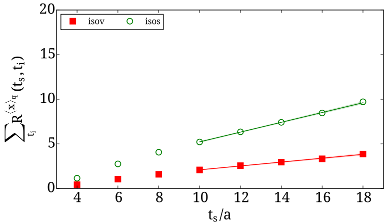
✗ Excited states enter as max $e^{-\Delta(t_s - t_{\text{ins}})}$, $e^{-\Delta t_{\text{ins}}}$

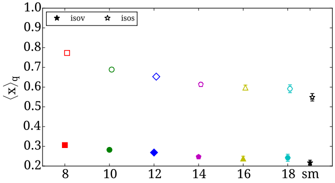


Fit to summed ratio

✓ Excited states enter as $e^{-\Delta t_s}$

✗ Two parameter fit: cross-correlations between fit parameters ⇒ larger uncertainties





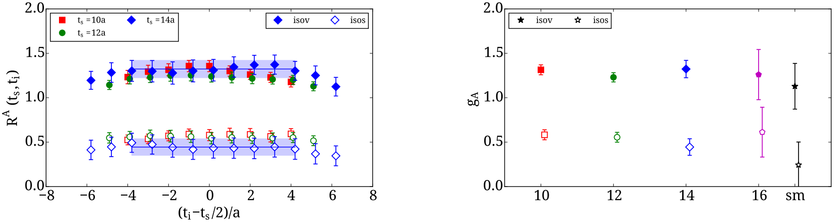
- Example a lattice with $m_\pi \simeq 370$ MeV
- t_s available from 0.7 - 1.5 fm
- Fit to excited states not always possible
- Ideally, matrix element value and error confirmed by all available methods

Nucleon axial charge g_A

- Isovector axial charge, from isovector axial vector current:

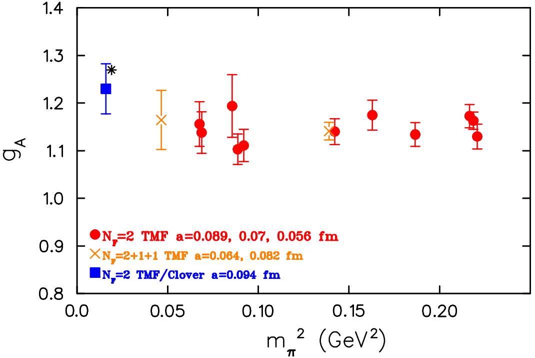
$$\mathcal{O}^{\mu}_{A3} = \bar{u}\gamma_5\gamma_\mu u - \bar{d}\gamma_5\gamma_\mu d \rightarrow \bar{v}_N(\mathbf{p}') \left[\gamma_5\gamma_\mu G_A(q^2) + \frac{q^\mu}{2m}\gamma_5 G_p(q^2)\right] v_N(\mathbf{p}),$$

- $g_A = G_A(0)$, isovector combination $\Rightarrow$ no quark-loops at $m_u = m_d$ limit
- Directly accessible at $q^2{=}0$



- Also showing connected isoscalar case: $\bar{u}\gamma_5\gamma_\mu u + \bar{d}\gamma_5\gamma_\mu d$
- Physical point lattice: $m_\pi = 0.135$ GeV, a=0.094 fm, $48^3 \times 96$
- $\sim$1,500 configurations analyzed
- No detectable excited state effects while varying t_s between 0.94-1.3 fm

Nucleon axial charge g_A



- Several lattice groups with simulations at near physical pion mass
- Increased statistics required due to increased noise-to-signal ratio at physical point [scales as $e^{m_N - \frac{3}{2} m_\pi}$]
- Dedicated study at physical point will require three lattice spacings, at least two volumes

- Twisted mass, $N_f = 2$, C. Alexandrou *et al.* arXiv:1012.0857, 1411.3494
  Twisted mass, $N_f = 2 + 1 + 1$, C. Alexandrou *et al.* arXiv:1303.5979
- $N_f = 2$ clover, G. Bali *et al.* arXiv:1412.7336; $N_f = 2 + 1$ DWF, T. Yamazaki *et al.* arXiv:0904.2039; $N_f = 2 + 1$ DWF on a staggered sea, LHPC arXiv:1001.3620; $N_f = 2 + 1$ clover, Green *et al.* arXiv:1209.1687

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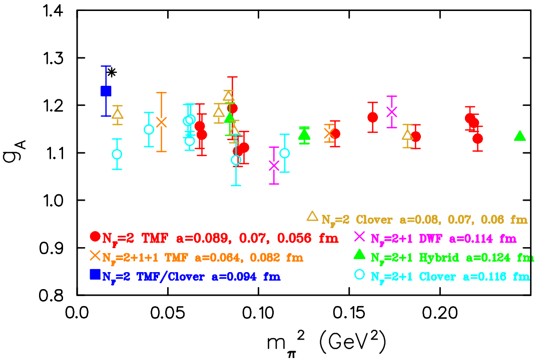

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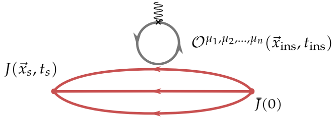
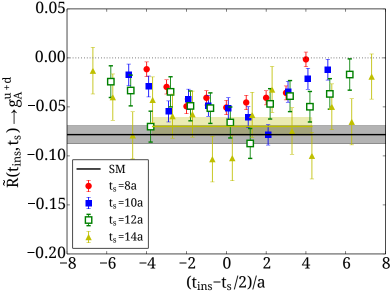
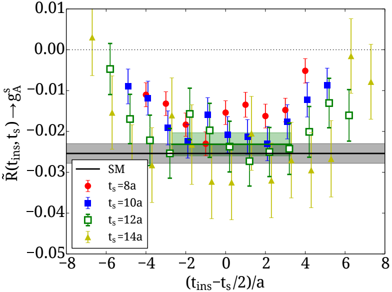
Nucleon axial charge g_A

- Disconnected quark loop contributions
- Contribute to isoscalar combinations of u- and d-quark currents.
- s-quark contributions to nucleon matrix elements







- Dedicated methods for stochastic evaluation of disconnected fermion loops
  A. Abdel-Rehim, C. Alexandrou, M. Constantinou, V. Drach, K. Hadjiyiannakou, K. Jansen, G. K., A. Vaquero `arXiv:1310.6339`
- 150,000 statistics at $m_\pi \simeq$370 MeV, $O(10^2)$ more than connected
- Contributions needed to isolate intrinsic nucleon spin contribution of individual u-, d- and s-quarks

Tensor charge

- Isovector tensor charge:

$$\mathcal{O}^{\mu\nu}_{T3} = \bar{u}\sigma_{\mu\nu}u - \bar{d}\sigma_{\mu\nu}d \to \bar{v}_N(\mathbf{p}')\left[\sigma_{\mu\nu}A_{T10}(q^2) + \frac{\gamma^{[\mu}\Delta^{\nu]}}{2m}B_{10}(q^2) + \frac{P^{[\mu}\Delta^{\nu]}}{m^2}\tilde{A}_{T10}(q^2)\right]v_N(\mathbf{p}),$$

$g_T = A_{T10}(0)$

- Ultra-cold neutron decay experiments for BSM
- Consistency between lattice descritizations
- Excited state effects expected small, based on high-statistics analysis at 370 MeV pion mass
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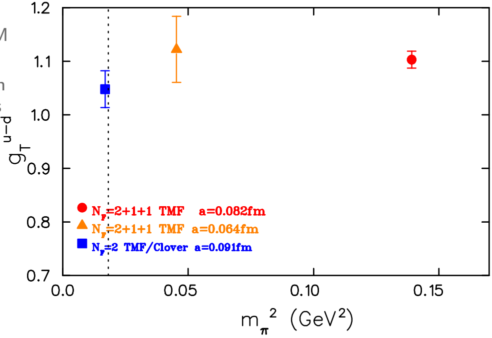

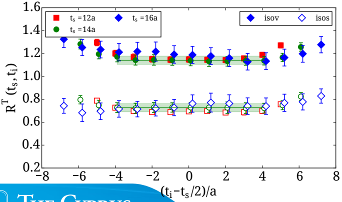

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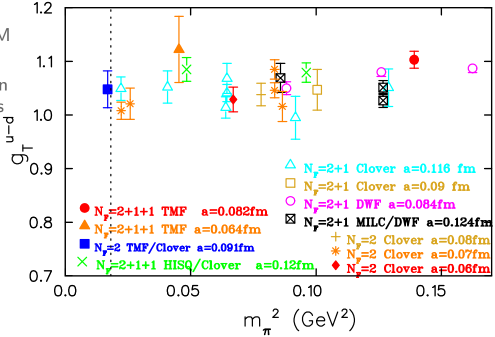
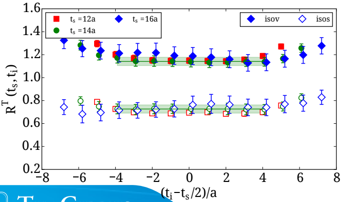




Nucleon electromagnetic form factors

— From vector current:

$$\mathcal{O}_V^\mu = \bar{u}\gamma_\mu u \pm \bar{d}\gamma_\mu d \to \bar{v}_N(\mathbf{p}') \left[\gamma_\mu F_1^{\overset{S}{V}}(q^2) + \frac{i\sigma_{\mu\nu} q^\nu}{2m} F_2^{\overset{S}{V}}(q^2) \right] v_N(\mathbf{p}),$$

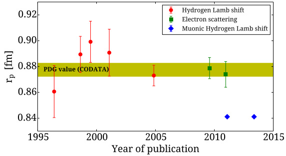
— Alternatively, the Electric (G_E) and (G_M) Sachs form factors:

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

— Radii (Dirac and Pauli) defined as slope at $Q^2 = 0$:

$$\langle r_i^2 \rangle = -\frac{6}{F_i} \frac{dF_i}{dQ^2}|_{Q^2=0}$$

similarly for $\langle r_E^2 \rangle$, $\langle r_M^2 \rangle$ (Electric and magnetic)

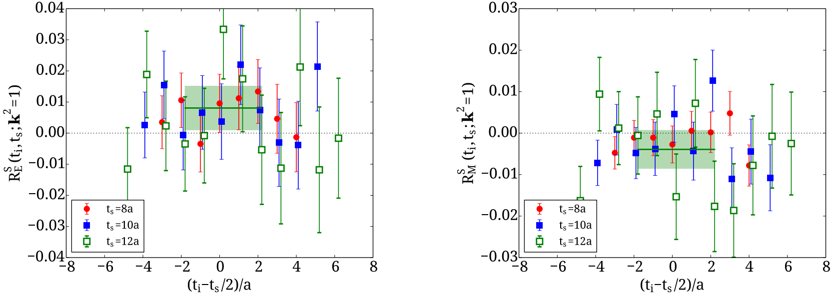


— Isovector and isoscalar combinations

- $j_{\mathrm{EM}}^\mu = \frac{2}{3}\bar{u}\gamma_\mu u - \frac{1}{3}\bar{d}\gamma_\mu d$
- $\langle p|j_{\mathrm{EM}}^\mu|p\rangle - \langle n|j_{\mathrm{EM}}^\mu|n\rangle = \langle p|\bar{u}\gamma_\mu u - \bar{d}\gamma_\mu d|p\rangle$ - Isovector (no quark loop contributions)
- $\langle p|j_{\mathrm{EM}}^\mu|p\rangle + \langle n|j_{\mathrm{EM}}^\mu|n\rangle = \frac{1}{3}\langle p|\bar{u}\gamma_\mu u + \bar{d}\gamma_\mu d|p\rangle$ - Isoscalar (quark loop contributions)
- $F^p - F^n = F^V$ assuming flavor SU(2) isospin symmetry,
- $F^p + F^n = \frac{1}{3}F^S$ i.e. $p \leftrightarrow n$ when $u \leftrightarrow d$

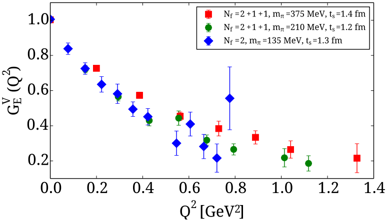
Nucleon electromagnetic form factors

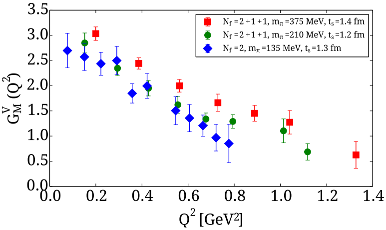
- Dedicated study of disconnected contribution arXiv:1310.6339

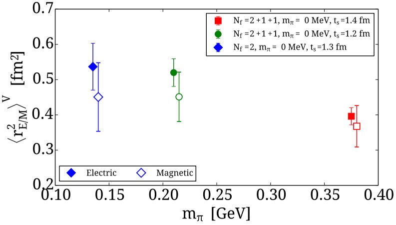


- Twisted mass $N_f = 2+1+1$, $a \simeq$0.085 fm, $m_\pi \simeq$370 MeV
- $\sim$150,000 statistics
- Connected contribution $O(1) \Rightarrow$ disconnected bound to $\sim$1% at this pion mass

Nucleon electromagnetic form factors





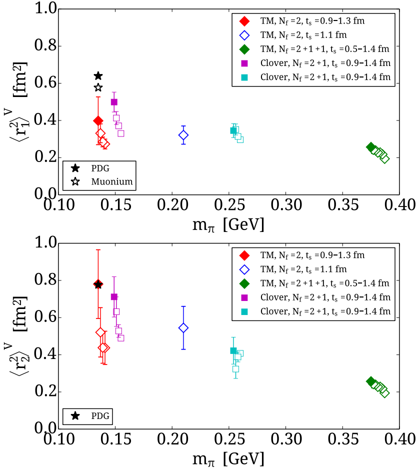


- Three ensembles of twisted mass fermions
- Physical point: $N_f = 2$, $a \simeq 0.094$ fm, $m_\pi \simeq 135$ MeV
  - $\sim$1,000 statistics for $t_s - t_0 = 1.1$ and 1.3 fm, $\sim$300 for 0.9 fm
- $t_s - t_0 > 1.2$ fm
- Tendency for steeper G_E and G_M as $m_\pi \to 135$ MeV $\Rightarrow$ larger radii
- Radii from fit to dipole forms:

$$F_1(Q^2) = \frac{1}{(1 + Q^2/M_1^2)^2}, \qquad \langle r_i^2 \rangle = \frac{12}{M_i^2}$$

$$F_2(Q^2) = \frac{F_2(0)}{(1 + Q^2/M_2^2)^2}$$

Nucleon electromagnetic form factors



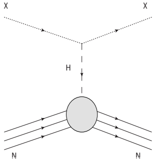
- Including LHPC data: `arXiv:1404.4029`
  - Clover improved, $a = 0.116$ fm, $m_\pi = 149$ MeV
  - Consistency between the two discretizations
- Curvature towards physical point
- Increasing trend for enlarging source-sink separation at near physical pion masses
- Need $\sim 1\%$ error to contact experiment, or a multiple-fold increase in statistics.

Nucleon σ-terms

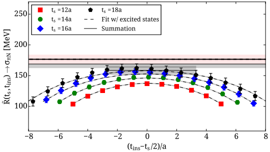
- Pion-nucleon (light) σ-term: $\sigma_{\pi N} = m_{ud}\langle N|\bar{u}u + \bar{d}d|N\rangle$
- Strange σ-term: $\sigma_s = m_s\langle N|\bar{s}s|N\rangle$
- Non negligible contribution from excited states
- Strange content:

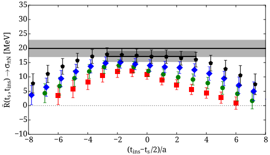
$$y_N = \frac{2\langle N|\bar{s}s|N\rangle}{\langle N|\bar{u}u + \bar{d}d|N\rangle} = 1 - \frac{\sigma_0}{\sigma_{\pi N}}$$

with $\sigma_0 = m_{ud}\langle N|\bar{u}u + \bar{d}d - 2\bar{s}s|N\rangle$



- Three estimates for $\sigma_{\pi N}$:
  45 ± 8 MeV (GLS);
  64 ± 7 MeV (GWU);
  59 ± 7 MeV (AMO);
- $\sigma_0 = 36 \pm 7$ MeV B. Borasoy and U.-G. Meissner
- $\sigma_0 = 58 \pm 8$ MeV J. Alarcon, L. Geng, J. Martin Camalich, and J. Oller
- Yields: y_N within 0.02 - 0.44 with at least 30% error
- Enters super-symmetric candidate particle scattering cross sections with nucleon (e.g. neutralino through Higgs)
  $\rightarrow$ First principles evaluation from the lattice





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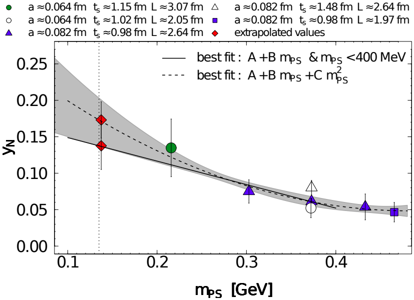
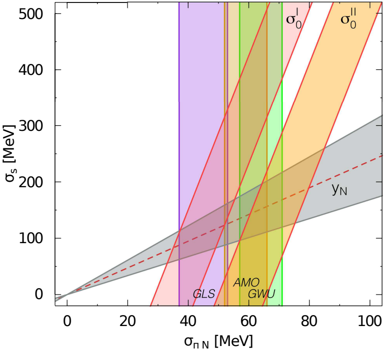
Nucleon σ-terms

C. Alexandrou *et al.* `arXiv:1309.7768`



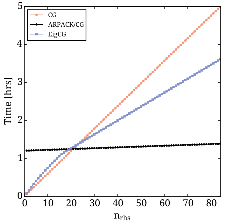
- Chiral extrapolation to physical pion mass
- $y_N = 0.173(29)(36)(19)(9)$
- Error budget includes excited states (source-sink separation), chiral fit, lattice spacing

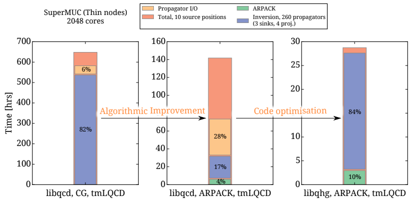


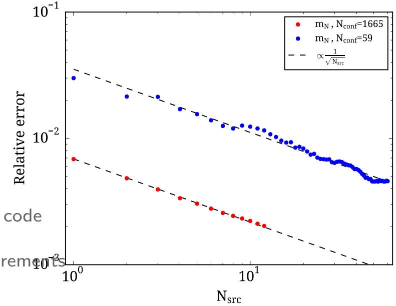
- Given y_N can infer constraints on $\sigma_{\pi N}$, σ_0

Noise reduction techniques

- Use multiple measurements per gauge-field configuration (e.g. multiple source locations)
- Statistically independent for large enough volumes
- Allows employing multiple right-hand-side solvers
- Exact deflation via a polynomially accelerated Arnoldi







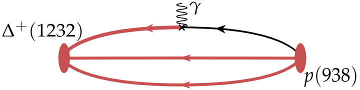
- Combination of both algorithmic improvements and code optimisation for multiple-fold run-time improvement
- Confirmed $1/\sqrt{N}$ error scaling with up to 64 measurements per configuration

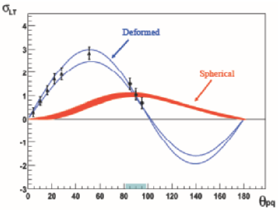
Nucleon to Δ electromagnetic transition

- Transition form factors:

$$\langle \Delta(p', s')| j^{\mu}_{\rm EM} | N(p, s)\rangle \rightarrow \bar{v}_\sigma(p', s') \left[G_{M1}(q^2) K^{\sigma\mu}_{M1} + G_{E2}(q^2) K^{\sigma\mu}_{E2} + G_{C2}(q^2) K^{\sigma\mu}_{C2} \right] v(p, s)$$

- Dominant magnetic dipole transition G_{M1}
- Subdominant
  - Electric quadrupole G_{E2}
  - Coulomb quadrupole G_{C2}
- Non-zero sub-dominants indicate an intrinsic quadrupole moment



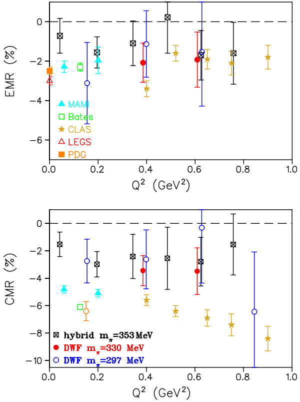


Experimentally used as probe for deformation in nucleon

C. N. Papanicolas, Eur. Phys. J. A18 (2003); N. Sparveris et al., PRL 94, 022003 (2005)

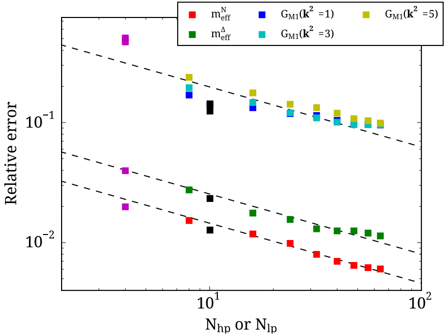
Nucleon to Δ electromagnetic transition

C. Alexandrou *et al.* arXiv:1011.3233



- Large uncertainties for sub-dominants from the lattice
- However consistently negative and non-zero

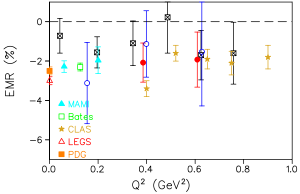
With USQCD group @ MIT

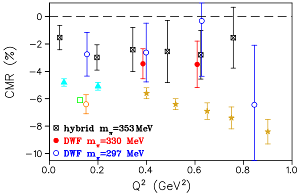


- Domain Wall configurations by the RBC collaboration
- New methods for efficiently calculating correlation functions at near-physical pion mass
- $m_\pi = 180$ MeV Domain Wall fermions
- All-mode-averaging for 64 measurements per gauge configuration
- 100 gauge configurations $\rightarrow$ 6,400 statistics

Nucleon to Δ electromagnetic transition

C. Alexandrou *et al.* `arXiv:1011.3233`





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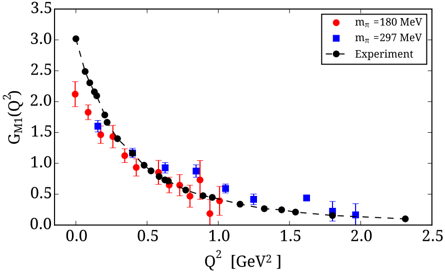

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Summary

- **LQCD benchmark quantities**
  - A number of lattice QCD calculations at physical pion mass
  - Multiple lattice spacings and volumes required for removing all systematic uncertainties
- **Need improved methods for efficiently increasing statistics at physical point**
  - Multiple right-hand-side linear solvers
  - Disconnected diagram calculations possible thanks to new computer technologies (e.g. GPUs) and methods
- **Paves the way towards precision nucleon structure calculations**
  - First pin down benchmark quantities, e.g. g_A, $\langle x \rangle$
    $\rightarrow$ Confidence in precision matrix element calculations
  - Multiple observables in the pipeline: σ-terms, tensor charge, EM form-factors

Thank you!

A. Abdel-Rehim, C. Alexandrou, M. Constantinou, S. Dinter, V. Drach, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, J. Negele, M. Petschlies, A. Strelchenko, A. Vaquero

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— SuperMUC at LRZ
— Fermi at CINECA
— Minotauro at BSC

European Twisted Mass Collaboration

Configurations by the European Twisted Mass collaboration