Fundamental Symmetries in Lattice Low-Energy Nuclear Physics

INSTITUTE FOR NUCLEAR THEORY

Intersections of BSM Phenomenology and QCD for New Physics Searches

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Low-Energy Nuclear Physics

- Understanding Nuclear Physics from QCD

- Testing the Standard Model at low-energy in nuclear environments

Low-Energy Nuclear Physics

- *Testing the Standard Model at low-energy in nuclear environments*
  - *Assuming CP-violating new physics from massive SM extension ($M_\Lambda > M_W$), what is the manifestation of this new physics at low-energy?*

Fundamental Symmetries and Low-Energy Nuclear Physics

- The Universe is matter dominated at roughly 1 ppb:

$$\eta \equiv \frac{X_{p+n}}{X_\gamma} = 6.19(15) \times 10^{-10}$$

- Sources of CP-violation beyond the Standard Model (SM) are needed to generate this observed asymmetry

- Assuming nature is CPT symmetric, this implies T-violation which implies fermions will have permanent electric dipole moments (EDMs)

- This has motivated significant experimental efforts to search (or plan to search) for permanent EDMs in a variety of systems

e, n, p, deuteron, triton, ^{3}He, ..., ^{199}Hg, ^{225}Ra, ^{229}Pa,...

Fundamental Symmetries and Low-Energy Nuclear Physics

- In order to interpret a measurement/constraint of an EDM in a nucleon or nuclei as a value/bound of couplings to BSM physics, we must have a solution to QCD in the IR

- Our tools of choice are lattice QCD (LQCD) and Effective Field Theory (EFT)

- We desire to compute completely a nucleon EDM resulting from CP violating operators, however, this is challenging and will take more time

- In the meantime, we can exploit symmetries (tricks) to determine the long-range CP-violating π-N couplings from simple spectroscopic LQCD calculations which are expected to dominate the EDMs of certain nuclei (eg ^{225}Ra)

- In a large nucleus, the long-range pion exchange will (may) dominate the nuclear EDM

$$\mathcal{L}_{CPV} = -\frac{\bar{g}_0}{2F_\pi}\bar{N}\vec{\pi}\cdot\vec{\tau}N - \frac{\bar{g}_1}{2F_\pi}\bar{N}\pi_3 N - \frac{\bar{g}_2}{2F_\pi}\pi_3\bar{N}\left(\tau_3 - \frac{\pi_3}{F_\pi}\vec{\pi}\cdot\vec{\tau}\right)N$$

- For the QCD theta term

$$\{\bar{g}_1, \bar{g}_2\} \sim \bar{g}_0\frac{m_\pi^2}{\Lambda_\chi^2}$$

- For more generic CP Violating operators

$$\bar{g}_2 \sim \{\bar{g}_0, \bar{g}_1\}\frac{m_\pi^2}{\Lambda_\chi^2} \qquad \bar{g}_1 \sim \bar{g}_0$$

- The nuclear EDM is proportional to the Schiff moment

$$S = \sum_{i \neq 0} \frac{\langle \Phi_0 | S_z | \Phi_i \rangle \langle \Phi_i | H_{CPV} | \Phi_0 \rangle}{E_0 - E_i} + c.c.$$

$$S = \frac{2 M_N g_A}{F_\pi} \left(a_0 \bar{g}_0 + a_1 \bar{g}_1 + a_2 \bar{g}_2 \right)$$

- The Schiff parameters $\{a_0, a_1, a_2\}$ are computed with nuclear models under the assumption the CPV operator does not significantly distort the nuclear wave-function

- For a QCD theta term only $\bar{g}_1 \sim \bar{g}_2 \sim 0$ and thus a constraint on $\bar{\theta}$ can be made through the relation

$$\bar{g}_0 = \frac{\delta M_{n-p}^{m_d - m_u}}{m_d - m_u} \frac{2 m_d m_u}{m_d + m_u} \bar{\theta} = \alpha \frac{2 m_d m_u}{m_d + m_u} \bar{\theta}$$

- The nuclear EDM is proportional to the Schiff moment

$$S = \sum_{i \neq 0} \frac{\langle \Phi_0 | S_z | \Phi_i \rangle \langle \Phi_i | H_{CPV} | \Phi_0 \rangle}{E_0 - E_i} + c.c.$$

$$S = \frac{2 M_N g_A}{F_\pi} \left(a_0 \bar{g}_0 + a_1 \bar{g}_1 + a_2 \bar{g}_2 \right)$$

- ^{225}Ra is interesting nucleus as it is octupole deformed
  - "stiff" core making nuclear model calculations more reliable
  - nearly degenerate parity partner state

$$E^{-}_{1/2} - E^{+}_{1/2} = 55 \text{ KeV}$$

  - $10^2 - 10^3$ enhancement of $\{a_0, a_1, a_2\}$

- Sources of CP-Violation in quark sector:

Operator	[Operator]	No. Operators
$\bar{\theta}$	4	1
quark EDM	6	2
quark Chromo-EDM	6	2
Weinberg (GGG)	6	1
4-quark	6	2
4-quark induced	6	1

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$$\mathcal{L}_{CPV} = -\frac{g_s^2 \bar{\theta}}{32\pi^2} \tilde{G}_{\mu\nu} G^{\mu\nu} - \frac{i}{2} \bar{q} \sigma^{\mu\nu} \gamma_5 \left(\tilde{d}_0 + \tilde{d}_3 \tau_3 \right) G_{\mu\nu} q$$

$$\mathcal{L}_{CPV} = -\frac{\bar{g}_0}{2F_\pi} \bar{N} \vec{\pi} \cdot \vec{\tau} N - \frac{\bar{g}_1}{2F_\pi} \bar{N} \pi_3 N - \frac{\bar{g}_2}{2F_\pi} \pi_3 \bar{N} \left(\tau_3 - \frac{\pi_3}{F_\pi} \vec{\pi} \cdot \vec{\tau} \right) N$$

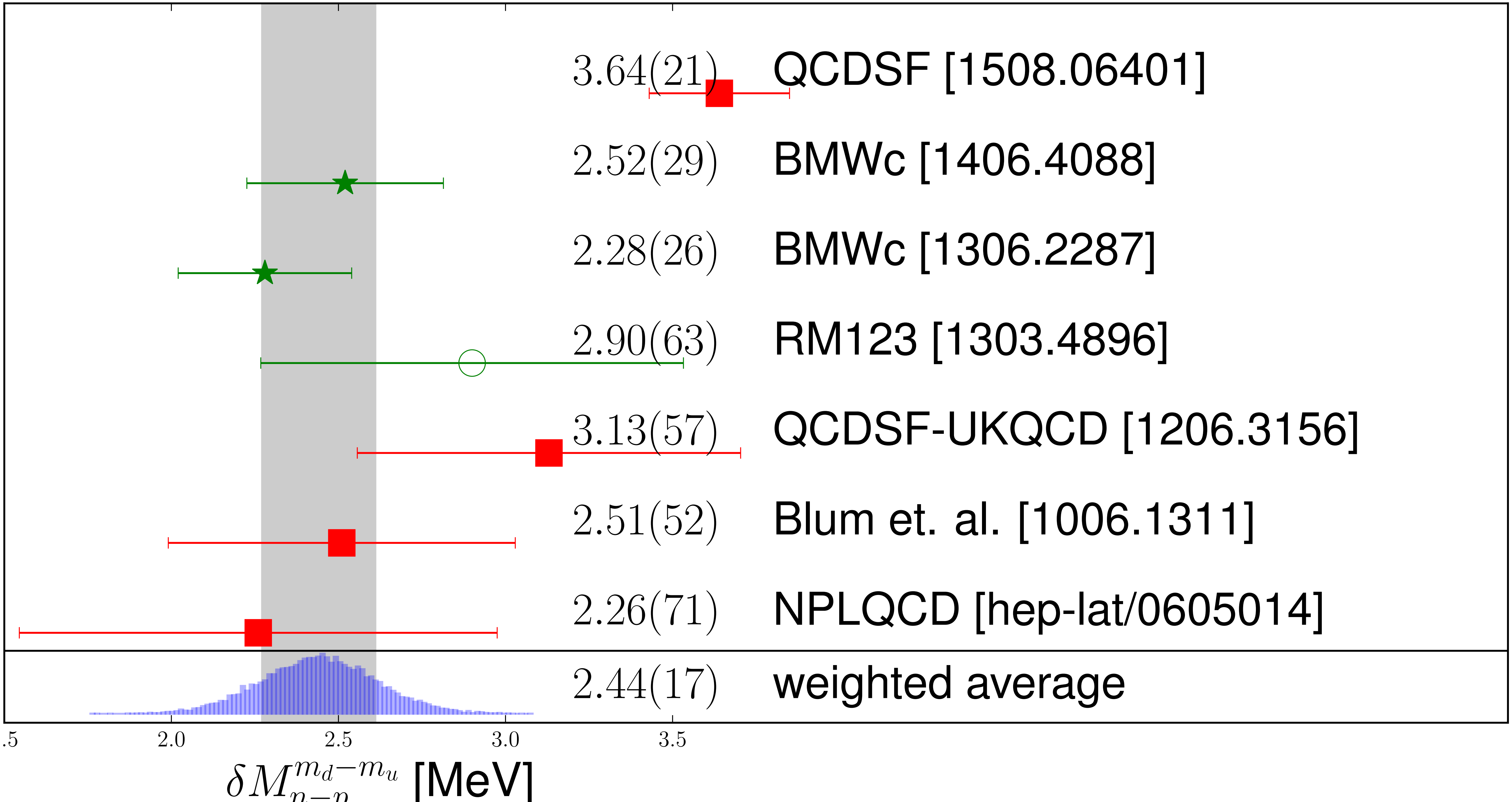
QCD Isospin Violation and CP-violating π-N

- A precise determination of the strong isospin breaking contribution to Mn-Mp teaches us about CP-violation (I learned all this from Emanuele Mereghetti)

$$\bar{g}_0 = \frac{\delta M_{n-p}^{m_d - m_u}}{m_d - m_u} \frac{2 m_d m_u}{m_d + m_u} \bar{\theta} = \alpha \frac{2 m_d m_u}{m_d + m_u} \bar{\theta}$$

Isospin Violation and Lattice QCD

- $\delta M_{n-p}^{m_d - m_u} = 2.44(17)$ MeV



Isospin Violation and Lattice QCD

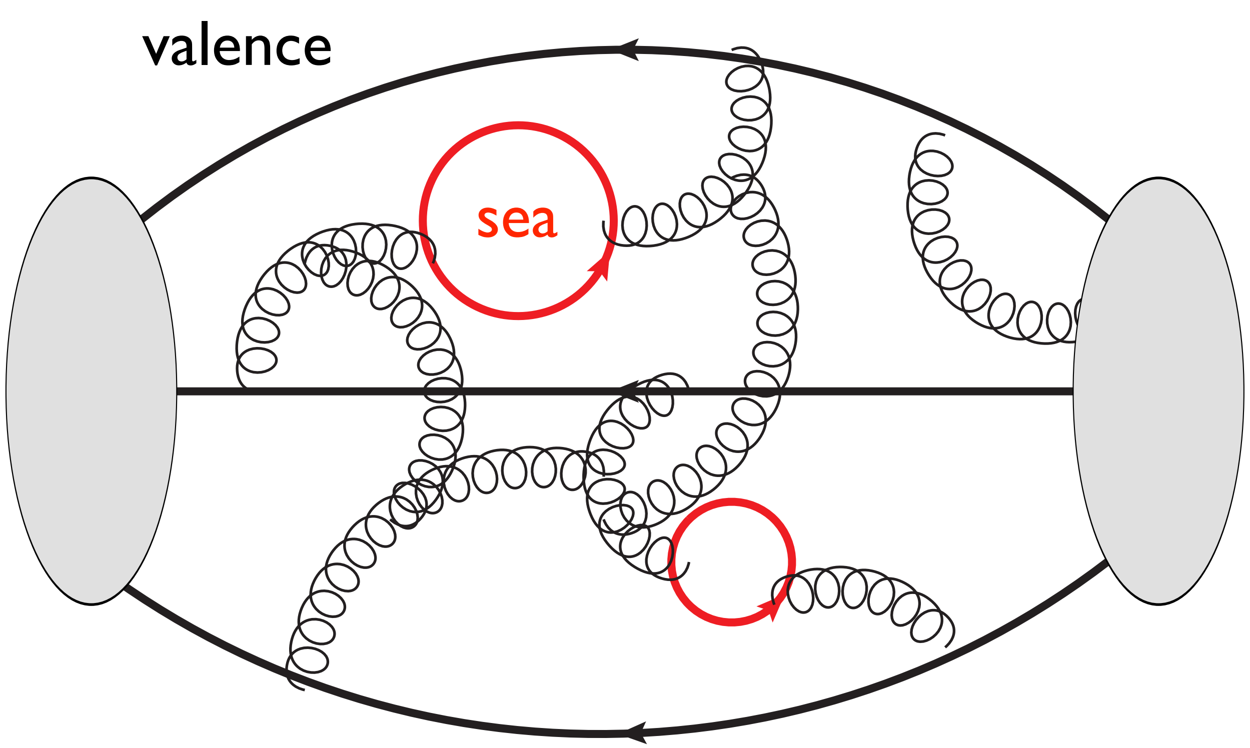
strong isospin breaking correction

$$\delta M_{n-p}^{m_d - m_u} = \alpha(m_d - m_u)$$

ideal problem for lattice QCD

$$\delta M_{n-p}^{m_d - m_u} = 2.44(17) \text{ MeV}$$

lattice average



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Beane, Orginos, Savage Nucl. Phys. B768 (2007)
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Blum, Izubuchi, etal Phys. Rev. D82 (2010)
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de Divitiis etal JHEP 1204 (2012)
Horsley etal Phys. Rev. D86 (2012)
de Divitiis etal Phys. Rev. D87 (2013)
Borsanyi etal arXiv:1306.2287
Borsanyi etal arXiv:1406.4088
Horsley etal arXiv:1508.06401

$$m_{u,d}^{valence} \neq m_l^{sea}$$

"partially quenched" lattice QCD trick that works on the computer but introduces error which must be corrected

Partially Quenched Nucleon Lagrangian

$$\mathcal{L}^{(PQ)} = \left(\overline{\mathcal{B}} v\cdot D \mathcal{B}\right) + \frac{\alpha_M^{(PQ)}}{(4\pi f)}\left(\overline{\mathcal{B}}\mathcal{B}\mathcal{M}_+\right) + \frac{\beta_M^{(PQ)}}{(4\pi f)}\left(\overline{\mathcal{B}}\mathcal{M}_+\mathcal{B}\right) + \frac{\sigma_M^{(PQ)}}{(4\pi f)}\left(\overline{\mathcal{B}}\mathcal{B}\right)\,\mathrm{tr}(\mathcal{M}_+)$$
$$- \left(\overline{\mathcal{T}}_\mu v\cdot D\,\mathcal{T}_\mu\right) - \Delta\left(\overline{\mathcal{T}}_\mu \mathcal{T}_\mu\right) + \frac{\gamma_M^{(PQ)}}{(4\pi f)}\left(\overline{\mathcal{T}}_\mu \mathcal{M}_+\mathcal{T}_\mu\right) - \frac{\overline{\sigma}_M^{(PQ)}}{(4\pi f)}\left(\overline{\mathcal{T}}_\mu\mathcal{T}_\mu\right)\mathrm{tr}(\mathcal{M}_+)$$
$$+ 2\alpha^{(PQ)}\left(\overline{\mathcal{B}}S^\mu\mathcal{B}A_\mu\right) + 2\beta^{(PQ)}\left(\overline{\mathcal{B}}S^\mu A_\mu\mathcal{B}\right) + 2\mathcal{H}^{(PQ)}\left(\overline{\mathcal{T}}^\nu S^\mu A_\mu \mathcal{T}_\nu\right) + \sqrt{\frac{3}{2}}\mathcal{C}\left[\left(\overline{\mathcal{T}}^\nu A_\nu\mathcal{B}\right) + \left(\overline{\mathcal{B}}A_\nu\mathcal{T}^\nu\right)\right]$$

$$\mathcal{L} = \overline{N}v\cdot DN + \frac{\alpha_M}{(4\pi f)}\overline{N}\mathcal{M}_+N + \frac{\sigma_M}{(4\pi f)}\overline{N}N\,\mathrm{tr}(\mathcal{M}_+)$$
$$+ \left(\overline{T}_\mu v\cdot D\,T_\mu\right) + \Delta\left(\overline{T}_\mu T_\mu\right) + \frac{\gamma_M}{(4\pi f)}\left(\overline{T}_\mu\mathcal{M}_+T_\mu\right) + \frac{\overline{\sigma}_M}{(4\pi f)}\left(\overline{T}_\mu T_\mu\right)\mathrm{tr}(\mathcal{M}_+)$$
$$+ 2\,g_A\,\overline{N}S\cdot A\,N - 2\,g_{\Delta\Delta}\,\overline{T}_\mu S\cdot A\,T_\mu + g_{\Delta N}\left[\overline{T}_\mu^{kji}A_i^{\mu,i'}\epsilon_{ji'}N_k + h.c.\right].$$

$$\alpha_M = \frac{2}{3}\alpha_M^{(PQ)} - \frac{1}{3}\beta_M^{(PQ)},$$
$$\sigma_M = \sigma_M^{(PQ)} + \frac{1}{6}\alpha_M^{(PQ)} + \frac{2}{3}\beta_M^{(PQ)},$$
$$\gamma_M = \gamma_M^{(PQ)}\ ,\ \bar{\sigma}_M = \bar{\sigma}_M^{(PQ)},$$

$$g_A = \frac{2}{3}\alpha^{(PQ)} - \frac{1}{3}\beta^{(PQ)}\ ,\ g_1 = \frac{1}{3}\alpha^{(PQ)} + \frac{4}{3}\beta^{PQ)},$$
$$g_{\Delta\Delta} = \mathcal{H}\ ,\ g_{\Delta N} = -\mathcal{C},$$

Isospin Violation and Lattice QCD

AWL arXiv:0904.2404

$$m^{val} = m^{sea} - \delta\tau_3$$

Nucleon Masses

$$M_n = M_0 + \frac{2B\delta}{4\pi f_\pi}\frac{\alpha_N}{2} + \frac{m_\pi^2}{4\pi f_\pi}\left(\frac{\alpha_N}{2} + \sigma_N(\mu)\right) - \frac{3\pi g_A^2}{(4\pi f_\pi)^2}m_\pi^3 - \frac{8g_{\pi N\Delta}^2}{3(4\pi f_\pi)^2}\mathcal{F}(m_\pi,\Delta,\mu) + \frac{3\pi\Delta_{PQ}^4(g_A+g_1)^2}{8m_\pi(4\pi f_\pi)^2}$$

$$M_p = M_0 - \frac{2B\delta}{4\pi f_\pi}\frac{\alpha_N}{2} + \frac{m_\pi^2}{4\pi f_\pi}\left(\frac{\alpha_N}{2} + \sigma_N(\mu)\right) - \frac{3\pi g_A^2}{(4\pi f_\pi)^2}m_\pi^3 - \frac{8g_{\pi N\Delta}^2}{3(4\pi f_\pi)^2}\mathcal{F}(m_\pi,\Delta,\mu) + \frac{3\pi\Delta_{PQ}^4(g_A+g_1)^2}{8m_\pi(4\pi f_\pi)^2}$$

Notice in the isospin splitting, not only the isospin violation appears as expected, but the non-analytic pion loop corrections exactly cancel, and the PQ effects exactly cancel! (This is only with "symmetric isospin breaking")

$$M_n - M_p = 2\alpha_N\delta\frac{B}{4\pi f_\pi} + \mathcal{O}(\delta^2, \delta m_\pi)$$

The expansion for M_n-M_p becomes similar to that of the pions (only even powers of the pion mass)

Full NNLO Nucleon mass splitting:

$$M_n - M_p = \frac{2B\delta}{4\pi f_\pi}\Bigg\{\alpha_N + \frac{m_\pi^2}{(4\pi f_\pi)^2}(b_1^M + b_6^M) + \frac{\mathcal{J}(m_\pi,\Delta,\mu)}{(4\pi f_\pi)^2} 4g_{\pi N\Delta}^2\left(\frac{5}{9}\gamma_M - \alpha_N\right)$$

$$\frac{m_\pi^2}{(4\pi f_\pi)^2}\left[\frac{20}{9}\gamma_M g_{\pi N\Delta}^2 - 4\alpha_N(g_A^2 + g_{\pi N\Delta}^2) - \alpha_N(6g_A^2+1)\ln\left(\frac{m_\pi^2}{\mu^2}\right)\right]$$

$$+ \frac{\alpha_N \Delta_{PQ}^4}{m_\pi^2(4\pi f_\pi)^2}\left(2 - \frac{3}{2}(g_A + g_1)^2\right)\Bigg\}$$

LQCD Calculation

PRELIMINARY

lattice QCD calculation performed using the Spectrum Collaboration anisotropic clover-Wilson gauge ensembles (developed @JLAB)

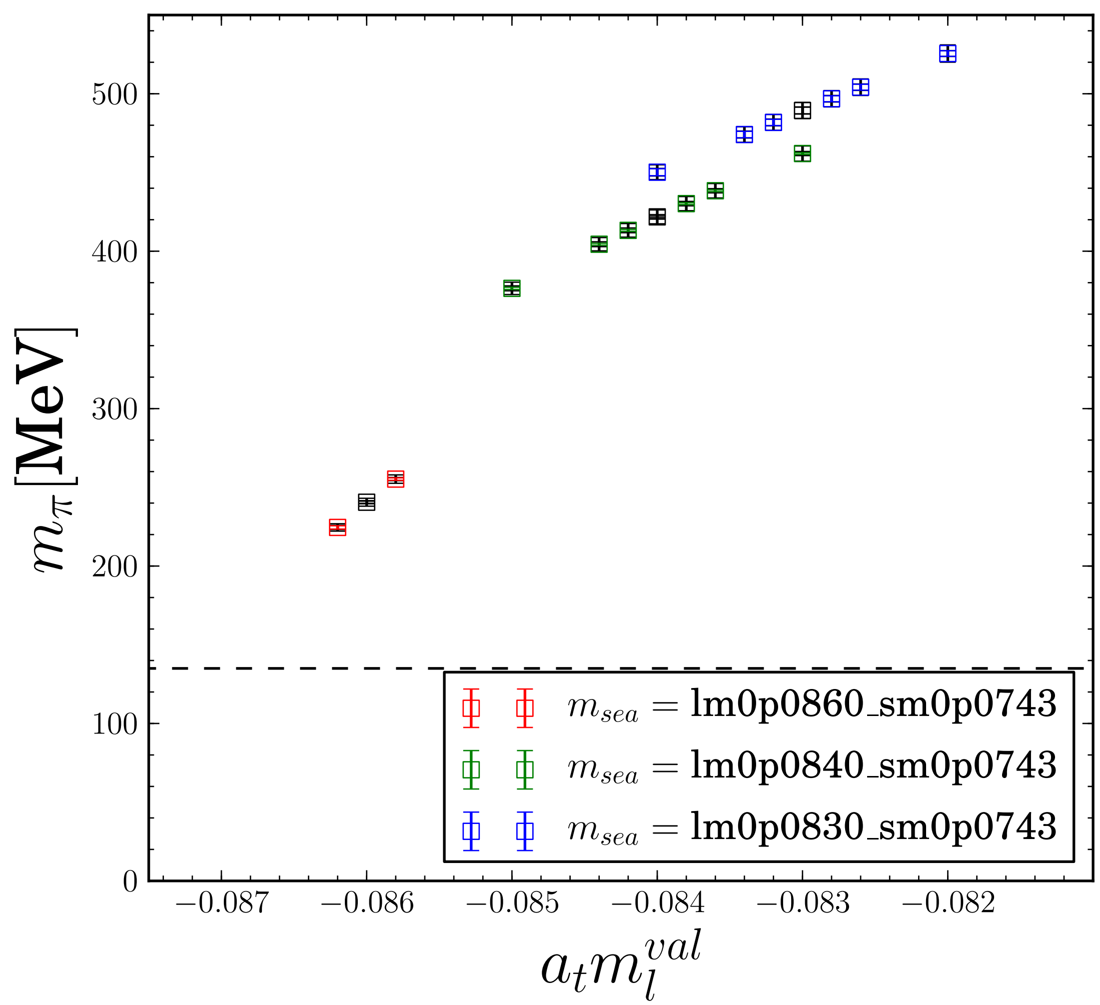
ensemble				$a_t m_\pi$	$a_t m_K$	$a_t\delta$ $[N_{cfg} \times N_{src}]$			
L	T	$a_t m_l$	$a_t m_s$			0.0002	0.0004	0.0010	0.0020
16	128	-0.0830	-0.0743	0.0800	0.1033	207×16	207×16	207×16	207×16
16	128	-0.0840	-0.0743	–	–	166×25	166×25	166×25	166×50
20	128	-0.0840	-0.0743	–	–	120×25	–	–	–
24	128	-0.0840	-0.0743	–	–	97×25	–	193×25	–
32	256	-0.0840	-0.0743	0.0689	0.0968	291×10	291×10	291×10	–
24	128	-0.0860	-0.0743	–	–	118×26	–	–	–
32	256	-0.0860	-0.0743	0.0393	0.0833	842×11	–	–	–

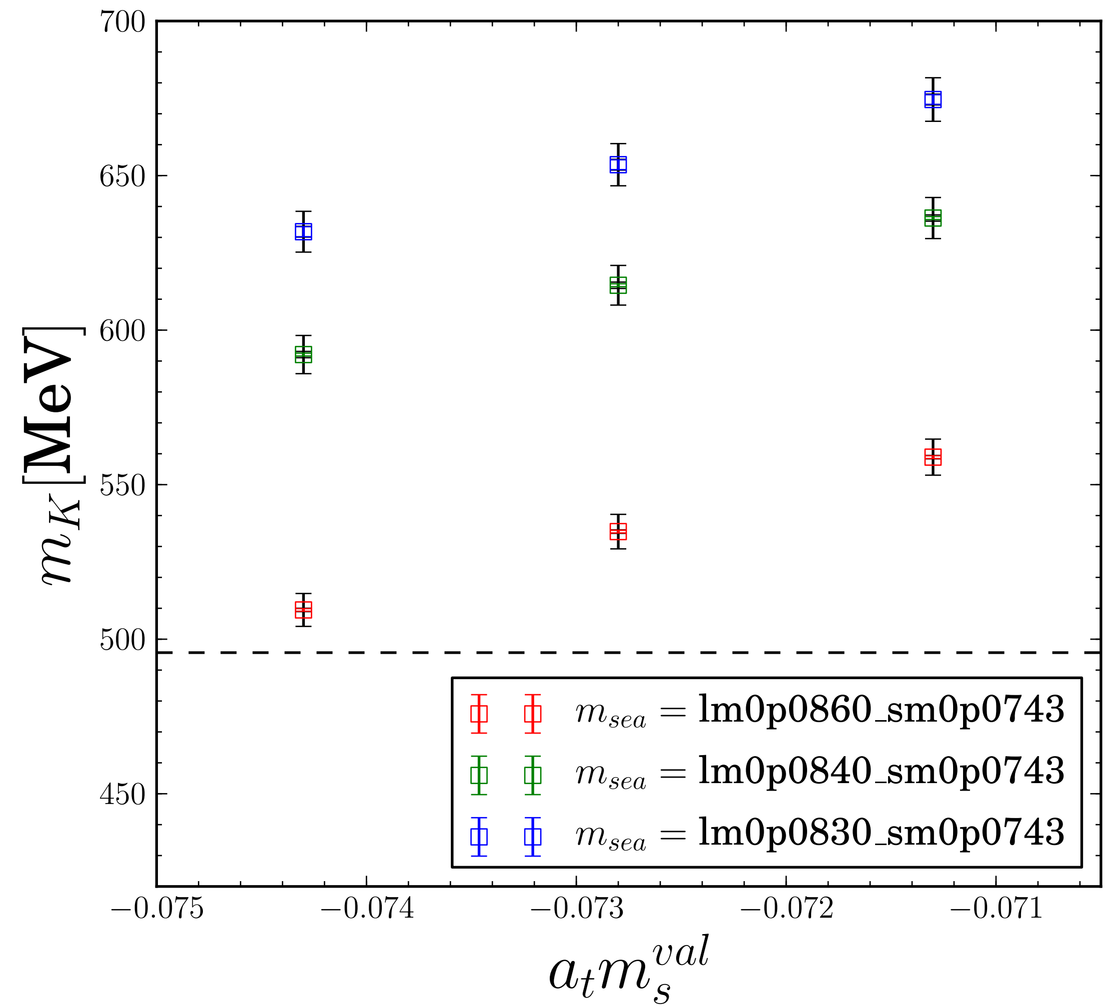
C.Aubin, W.Detmold,
E Mereghetti, K.Orginos,
S.Syritsyn, B.Tiburzi,
AWL

LQCD Calculation

Scale Setting

PRELIMINARY





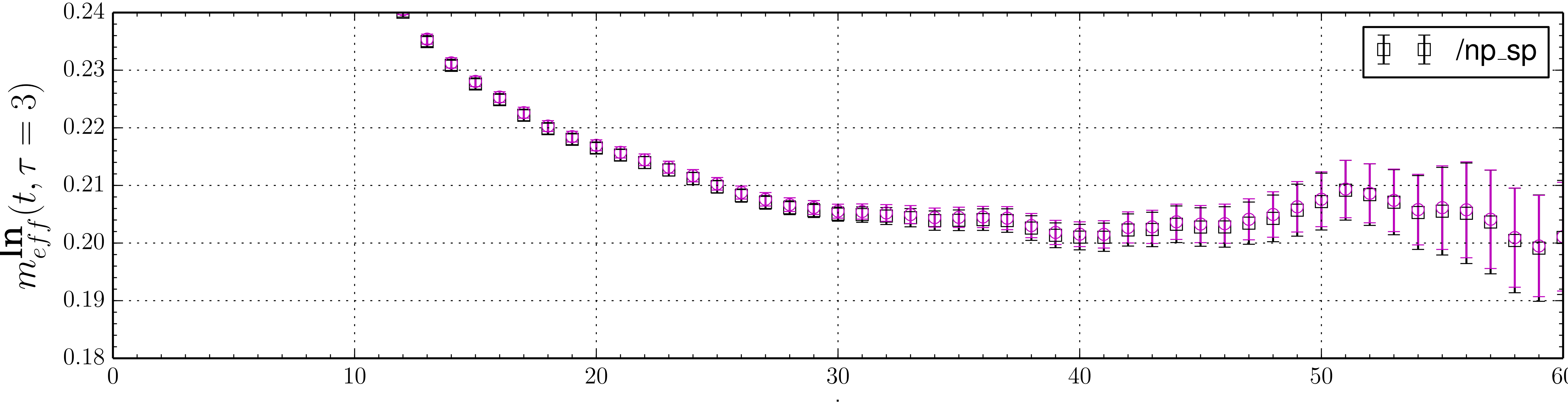
ensemble				m_π	m_K	$a_t\delta$ $[N_{cfg} \times N_{src}]$			
L	T	$a_t m_l$	$a_t m_s$	[MeV]	[MeV]	0.0002	0.0004	0.0010	0.0020
16	128	-0.0830	-0.0743	488	620	207×16	207×16	207×16	207×16
16	128	-0.0840	-0.0743	420	591	166×25	166×25	166×25	166×50
20	128	-0.0840	-0.0743	420	591	120×25	–	–	–
24	128	-0.0840	-0.0743	420	591	97×25	–	193×25	–
32	256	-0.0840	-0.0743	420	591	291×10	291×10	291×10	–
24	128	-0.0860	-0.0743	240	508	118×26	–	–	–
32	256	-0.0860	-0.0743	240	508	842×11	–	–	–

$$\delta^{latt}[\text{MeV}] = \begin{cases} 1.22 \\ 2.44 \\ 6.10 \\ 12.2 \end{cases}$$

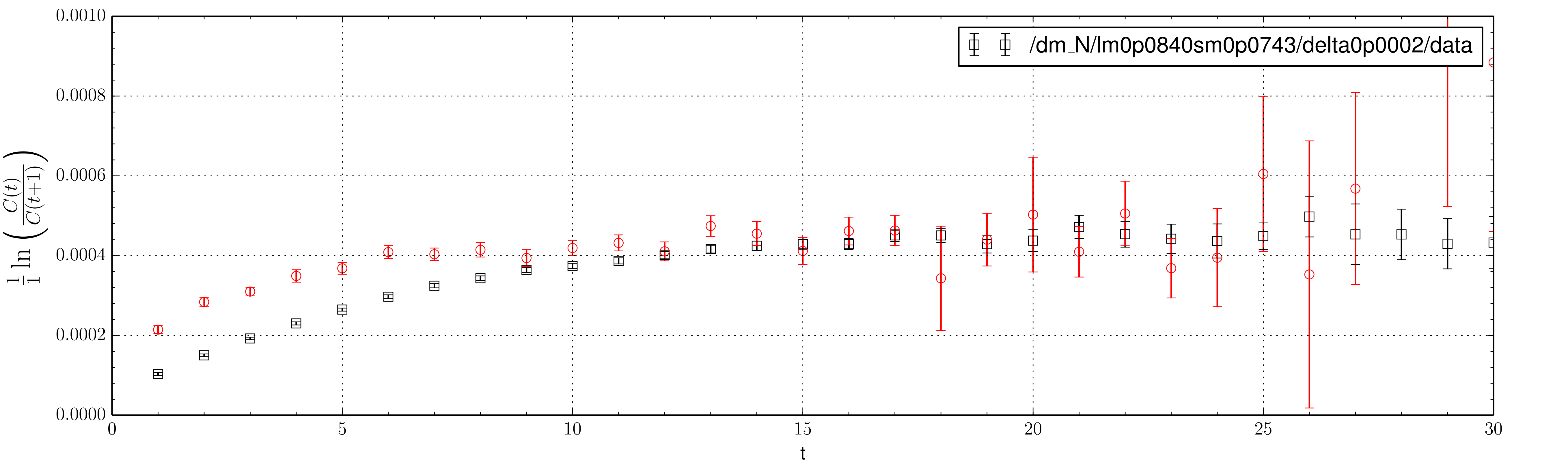
not renormalized

LQCD Calculation $M_n - M_p$ PRELIMINARY

Nucleon Mass Splitting



Ratio $C_n(t)$ / $C_p(t)$



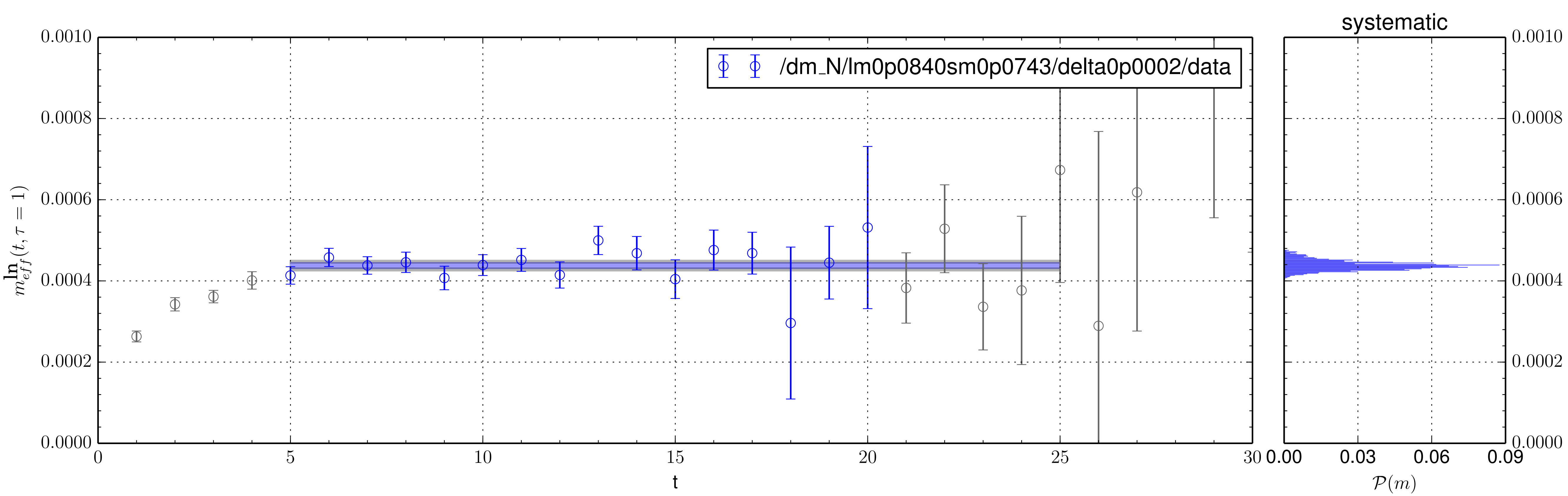
Nucleon Mass Splitting

Ratio $C_n(t)$ / $C_p(t)$

$$\frac{C_n(t)}{C_p(t)} = e^{-\delta M_N t} \frac{A_0 + \delta_0^n + (A_1 + \delta_1^n) e^{-(\Delta + \delta\Delta^n)t} + \cdots}{A_0 + \delta_0^p + (A_1 + \delta_1^p) e^{-(\Delta + \delta\Delta^p)t}}$$

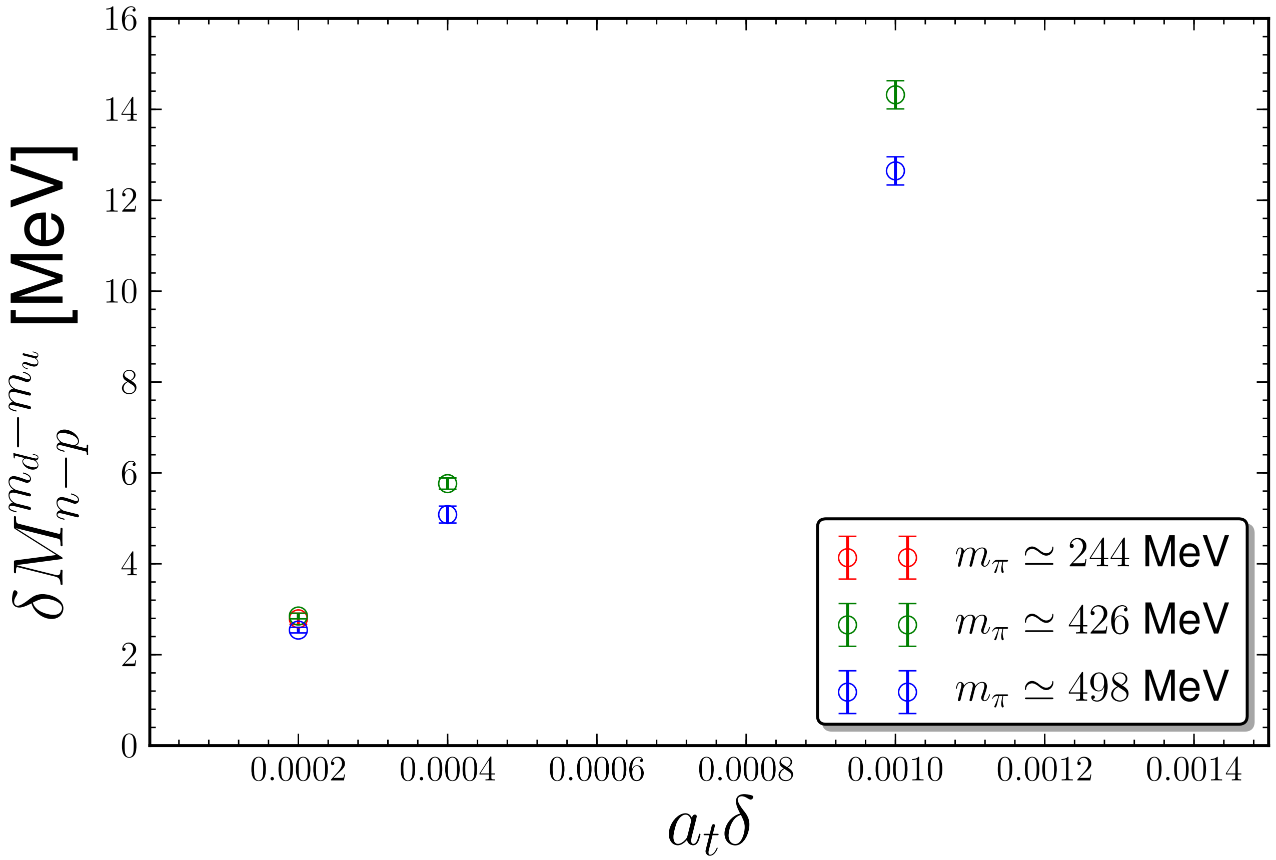
$$= e^{-\delta M_N t} \left\{ 1 + (\delta_0^n - \delta_0^p) + [\delta_1^n - \delta_1^p - A_1(\delta\Delta^n - \delta\Delta^p)t]\, e^{-\Delta t} \right\}$$

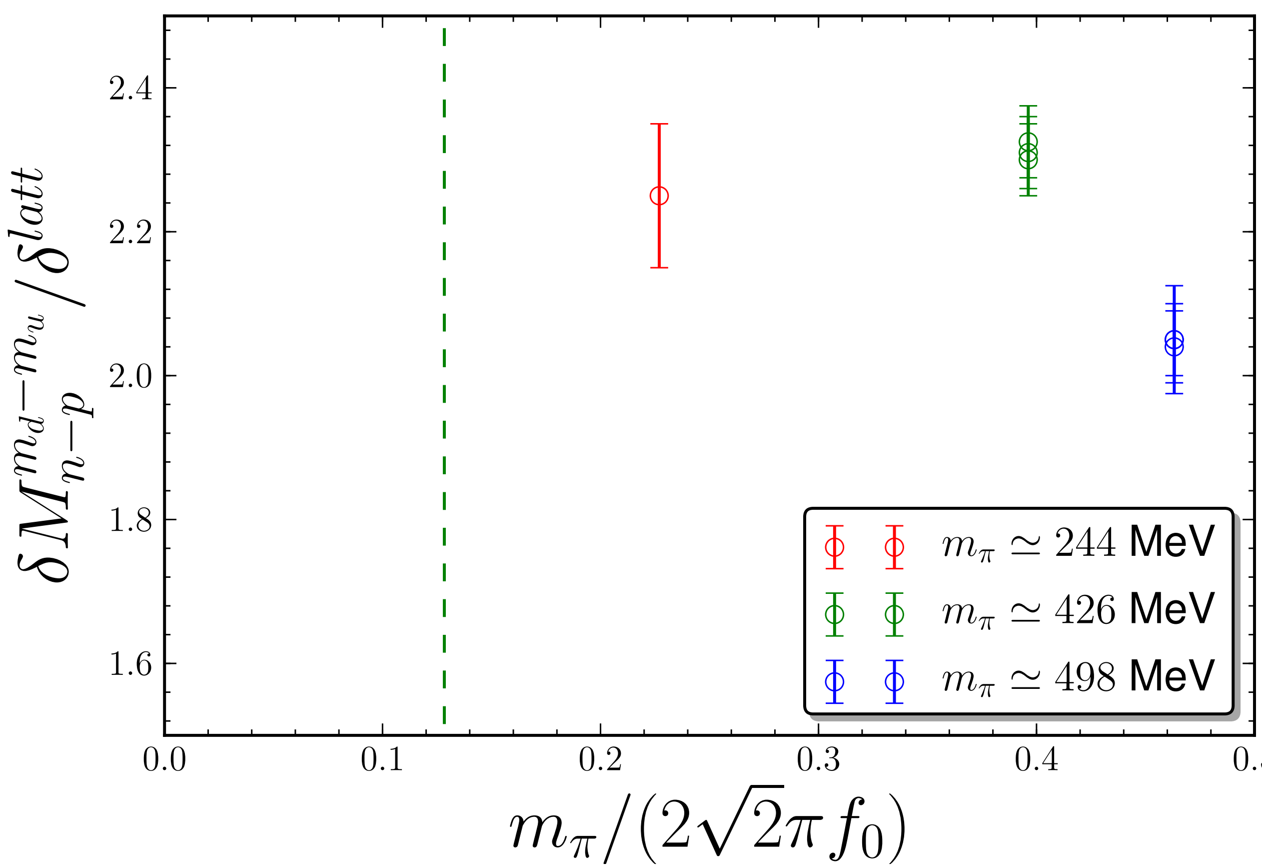
In ratio, excited state mass gap is the nucleon excited state, $\Delta >> M_n - M_p$



LQCD Calculation

PRELIMINARY



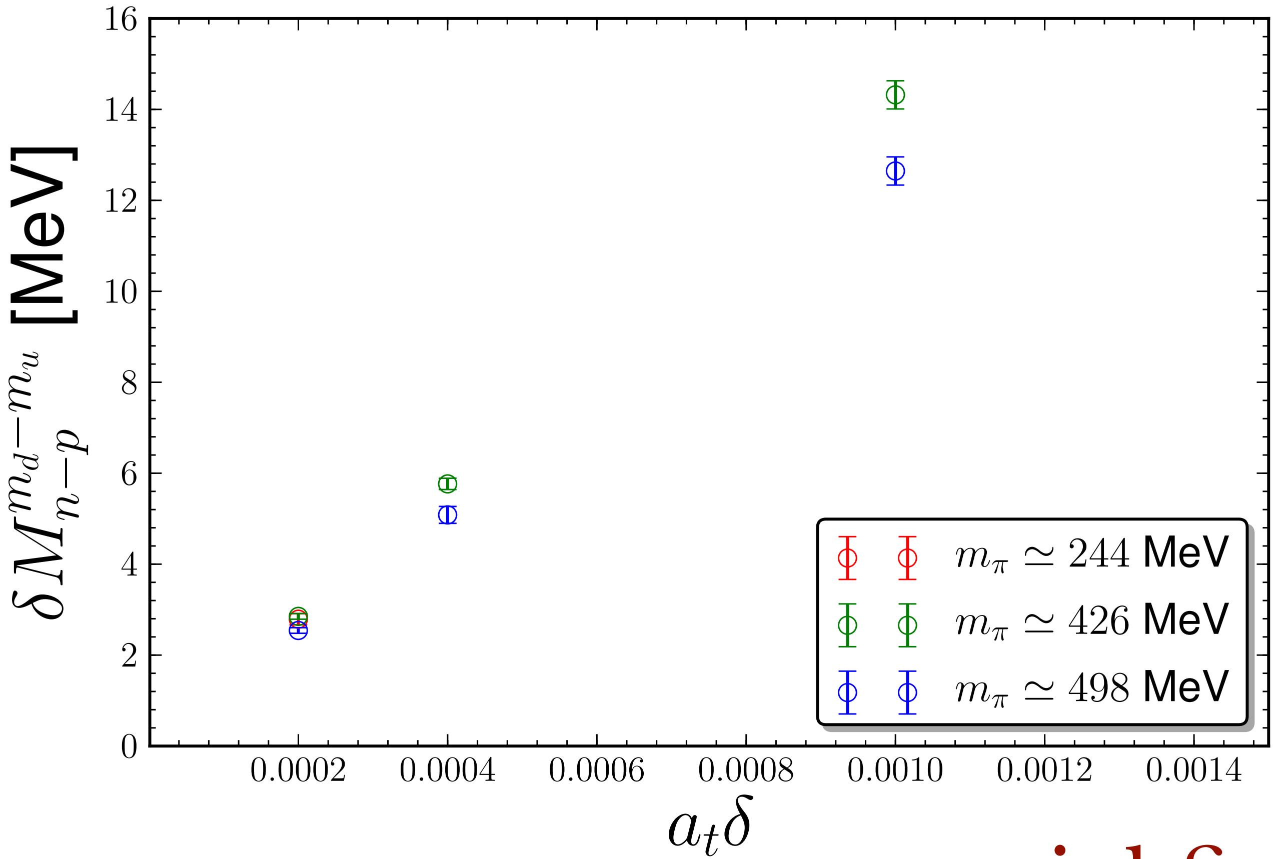


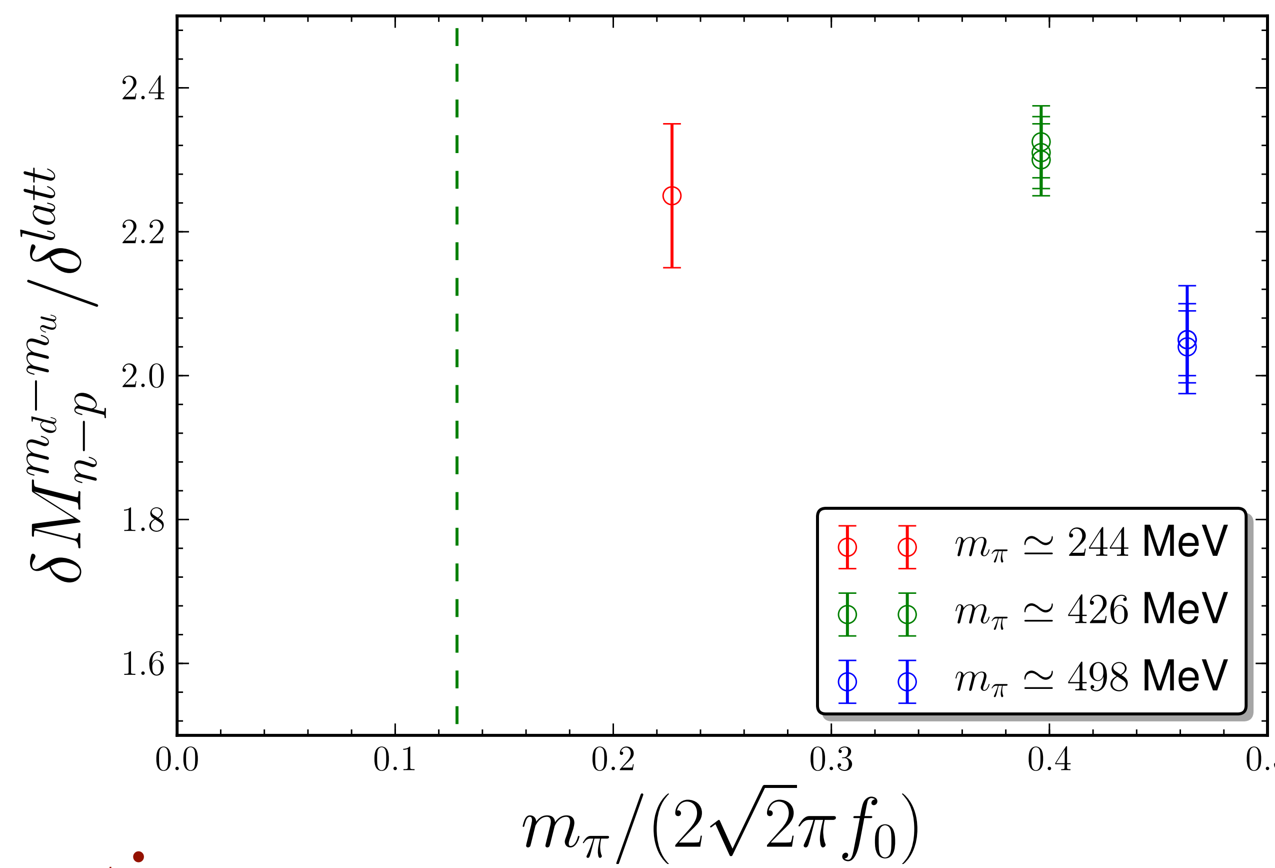
slope depends slightly on pion mass

no evidence for deviations from linear δ dependence

LQCD Calculation

PRELIMINARY





trial fit functions

polynomial in m_π^2

$$\delta M_{n-p}^{m_d-m_u} = \delta \left\{ \alpha + \beta \frac{m_\pi^2}{(4\pi f_\pi)^2} \right\}$$

$$\chi^2/dof = 13/5 = 2.6$$

NNLO χPT

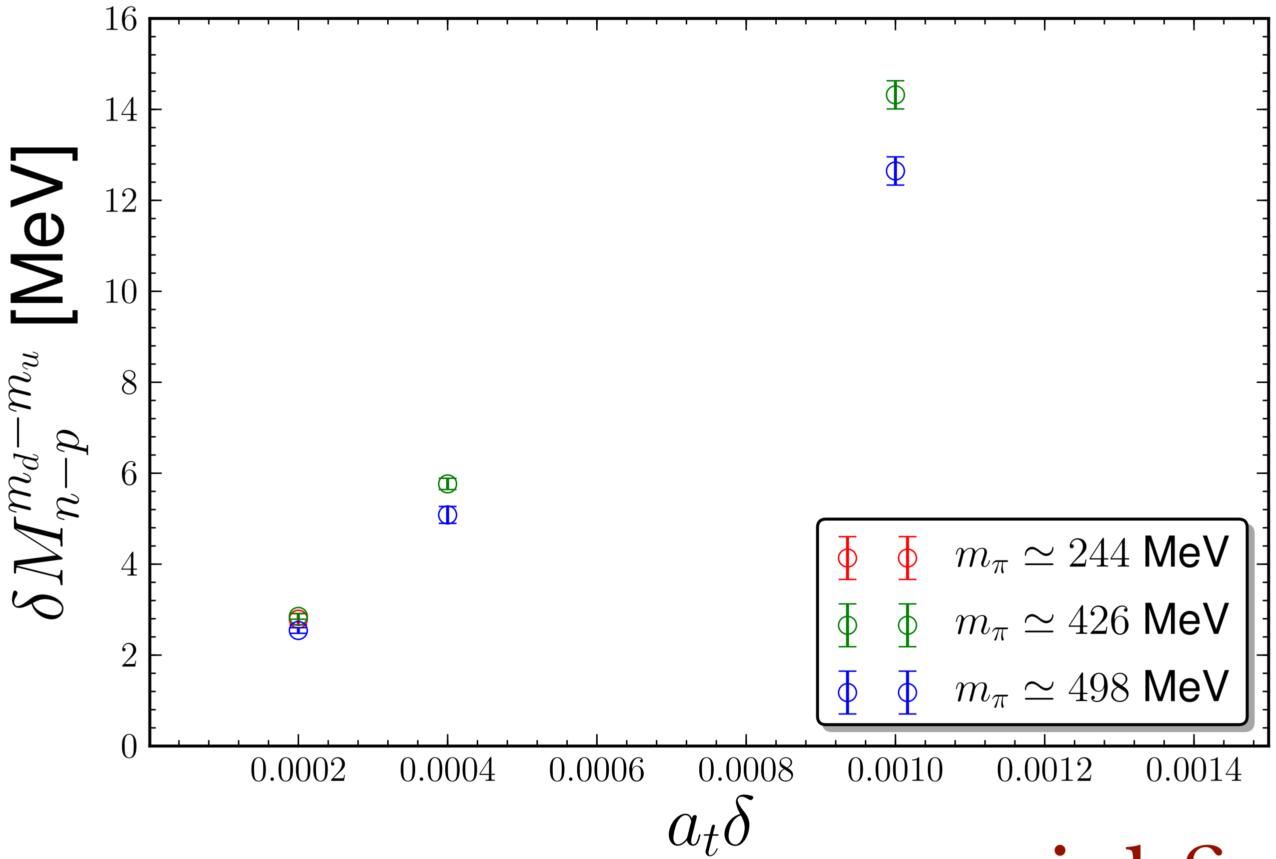
$$\delta M_{n-p}^{m_d-m_u} = \delta \left\{ \alpha \left[1 - \frac{m_\pi^2}{(4\pi f_\pi)^2}(6g_A^2+1)\ln\left(\frac{m_\pi^2}{\mu^2}\right) \right] + \beta(\mu)\frac{2m_\pi^2}{(4\pi f_\pi)^2} \right\}$$

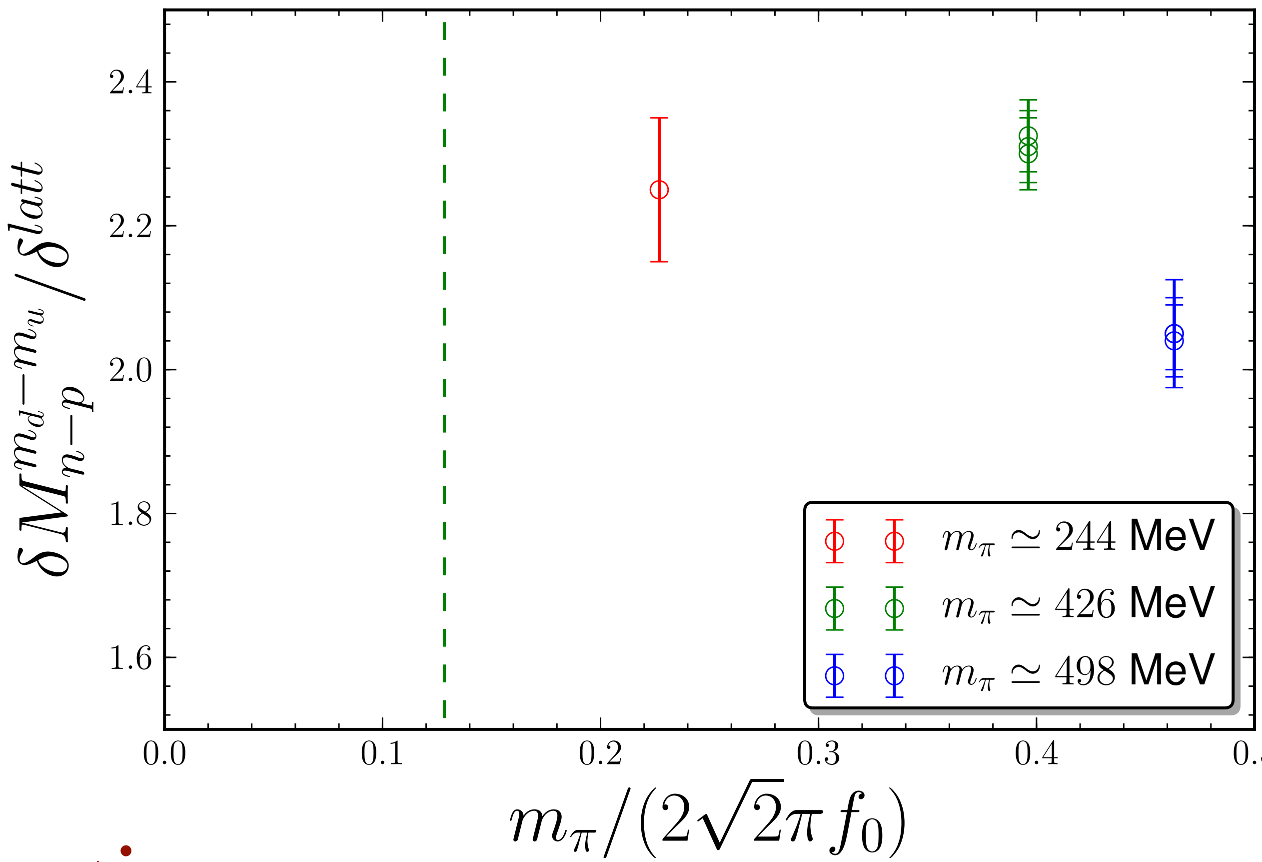
$(g_A = 1.27, f_\pi = 130\ \mathrm{MeV})$

$$\chi^2/dof = 1.66/5 = 0.33$$

LQCD Calculation

PRELIMINARY





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NNLO χPT

$$\delta M_{n-p}^{m_d-m_u} = \delta\left\{\alpha\left[1 - \frac{m_\pi^2}{(4\pi f_\pi)^2}(6g_A^2+1)\ln\left(\frac{m_\pi^2}{\mu^2}\right)\right] + \beta(\mu)\frac{2m_\pi^2}{(4\pi f_\pi)^2}\right\}$$

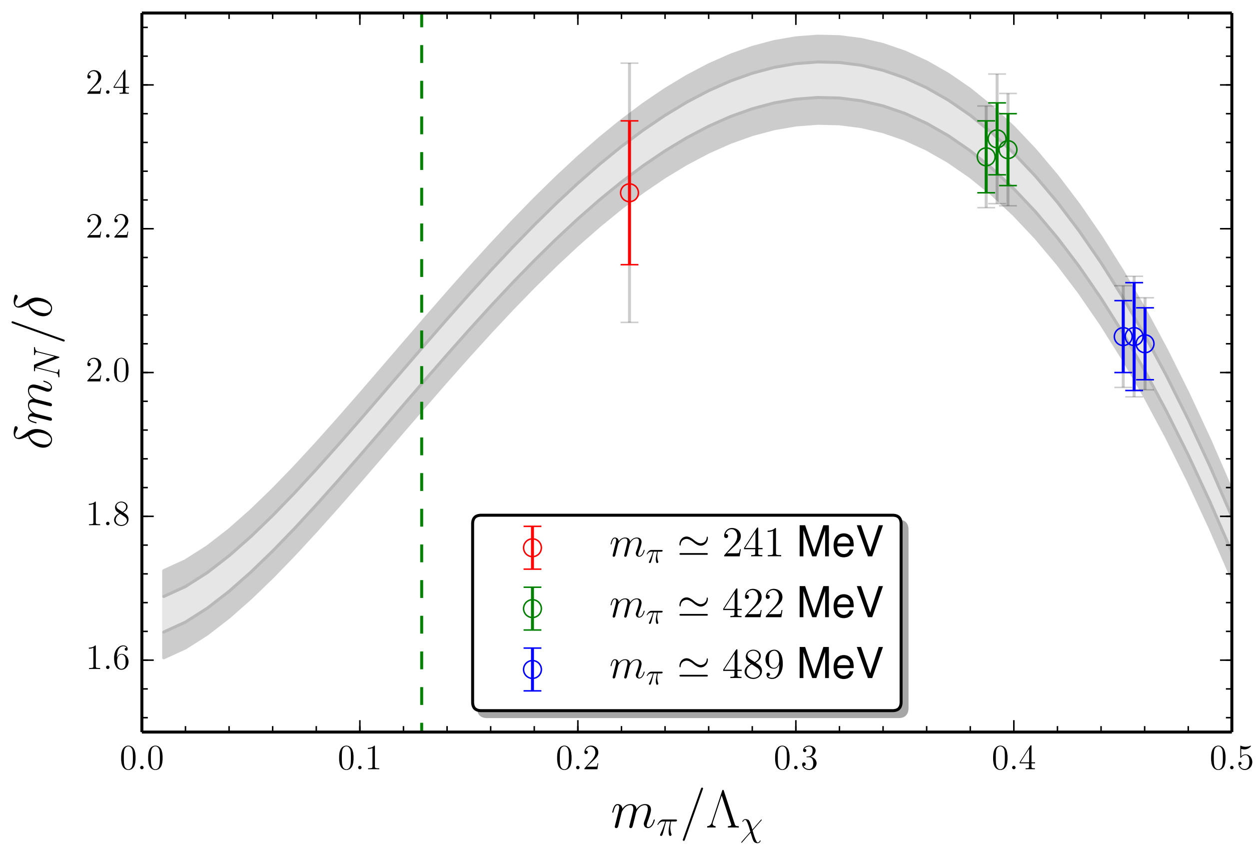
$(f_\pi = 130 \text{ MeV})$

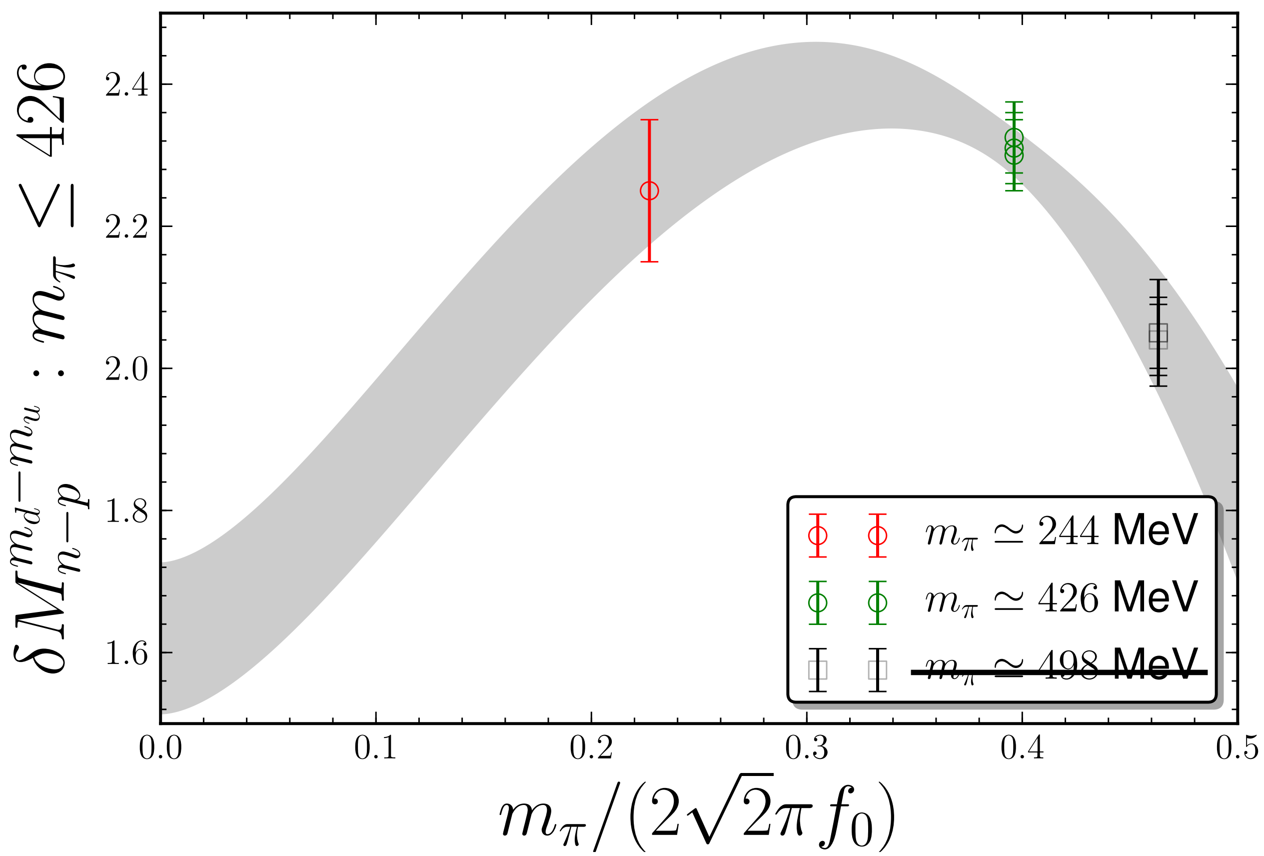
$$\chi^2/dof = 1.34/4 = 0.33$$

$\Rightarrow$ $g_A = 1.50(.29)$

LQCD Calculation

PRELIMINARY





NNLO χPT

$$\delta M_{n-p}^{m_d-m_u} = \delta\left\{\alpha\left[1 - \frac{m_\pi^2}{(4\pi f_\pi)^2}(6g_A^2+1)\ln\left(\frac{m_\pi^2}{\mu^2}\right)\right] + \beta(\mu)\frac{2m_\pi^2}{(4\pi f_\pi)^2}\right\}$$

$(g_A = 1.27, f_\pi = 130 \text{ MeV})$

$$\chi^2/dof = 1.66/5 = 0.33$$

exclude heavy mass point

this is striking evidence of a chiral logarithm

C.Aubin, W.Detmold, Emanuele Mereghetti, K.Orginos, S.Syritsyn, B.Tiburzi, AWL

Computational Strategy

- QCD Theta term

$$\mathcal{L}_{CPV} = -\frac{g_s^2\bar{\theta}}{32\pi^2}\tilde{G}_{\mu\nu}G^{\mu\nu} \quad \Rightarrow \quad \mathcal{L}^{\chi}_{CPV} = -\frac{\bar{g}_0}{2F_\pi}\bar{N}\vec{\pi}\cdot\vec{\tau}N$$

Symmetries $\Rightarrow$ $$\bar{g}_0 = \frac{\delta M_{n-p}^{m_d-m_u}}{m_d-m_u}\frac{2m_d m_u}{m_d+m_u}\bar{\theta}$$

$$\delta M_{n-p}^{m_d-m_u} = \alpha(m_d-m_u)$$

Simple spectroscopic calculation allows us to determine this long-range CP-Violating pion-nucleon coupling

This strategy was developed in conversations with Emanuele Mereghetti while we were both at LBNL

Computational Strategy

- Quark Chromo-EDM Operators

$$\mathcal{L}^{6}_{\bar{q}q} = -\frac{i}{2}\bar{q}\sigma^{\mu\nu}\gamma_5(\tilde{d}_0 + \tilde{d}_3\tau_3)G_{\mu\nu}q - \frac{1}{2}\bar{q}\sigma^{\mu\nu}(\tilde{c}_3\tau_3 + \tilde{c}_0)G_{\mu\nu}q$$

Computational Strategy

- Quark Chromo-EDM Operators

$$\mathcal{L}^6_{\bar{q}q} = -\frac{i}{2}\bar{q}\sigma^{\mu\nu}\gamma_5(\tilde{d}_0 + \tilde{d}_3\tau_3)G_{\mu\nu}q - \frac{1}{2}\bar{q}\sigma^{\mu\nu}(\tilde{c}_3\tau_3 + \tilde{c}_0)G_{\mu\nu}q$$

Symmetries ⇒

$$\bar{g}_0 = \delta_q M_N \frac{\tilde{d}_0}{\tilde{c}_3} + \delta M_N \frac{\Delta_q m_\pi^2}{m_\pi^2}\frac{\tilde{d}_3}{\tilde{c}_0}$$

$$\bar{g}_3 = -2\sigma_{\pi N}\left(\frac{\Delta_q M_N}{\sigma_{\pi N}} - \frac{\Delta_q m_\pi^2}{m_\pi^2}\right)\frac{\tilde{d}_3}{\tilde{c}_0}$$

Computational Strategy

- Quark Chromo-EDM Operators

$$\mathcal{L}^{6}_{\bar{q}q} = -\frac{i}{2}\bar{q}\sigma^{\mu\nu}\gamma_5(\tilde{d}_0 + \tilde{d}_3\tau_3)G_{\mu\nu}q - \frac{1}{2}\bar{q}\sigma^{\mu\nu}(\tilde{c}_3\tau_3 + \tilde{c}_0)G_{\mu\nu}q$$

Symmetries ⇒

$$\bar{g}_0 = \delta_q M_N \frac{\tilde{d}_0}{\tilde{c}_3} + \delta M_N \frac{\Delta_q m_\pi^2}{m_\pi^2}\frac{\tilde{d}_3}{\tilde{c}_0}$$

$$\bar{g}_3 = -2\sigma_{\pi N}\left(\frac{\Delta_q M_N}{\sigma_{\pi N}} - \frac{\Delta_q m_\pi^2}{m_\pi^2}\right)\frac{\tilde{d}_3}{\tilde{c}_0}$$

Again, all that is needed are simple spectroscopic quantities

$$\begin{aligned}
\delta M_N &= \text{nucleon mass splitting induced by } \mathcal{O} = \delta\,\bar{q}\,\tau_3\,q\,,\\
\sigma_{\pi N} &= \text{nucleon sigma-term induced by } \mathcal{O} = -\bar{m}\bar{q}q\,,\\
\delta_q M_N &= \text{nucleon mass splitting induced by } \mathcal{O} = -(\tilde{c}_3/2)\,\bar{q}\sigma^{\mu\nu}\tau_3 G_{\mu\nu}q\,,\\
\Delta_q M_N &= \text{nucleon sigma-term induced by } \mathcal{O} = -(\tilde{c}_0/2)\,\bar{q}\sigma^{\mu\nu}G_{\mu\nu}q\,,\\
\Delta_q m_\pi^2 &= \text{pion sigma-term induced by } \mathcal{O} = -(\tilde{c}_0/2)\,\bar{q}\sigma^{\mu\nu}G_{\mu\nu}q\,,
\end{aligned}$$

Computational Strategy

- Quark Chromo-EDM Operators

$$\mathcal{O}_0 = -\frac{1}{2}\bar{q}\sigma_{\mu\nu}G^{\mu\nu}q \qquad \mathcal{O}_3 = -\frac{1}{2}\bar{q}\tau_3\sigma_{\mu\nu}G^{\mu\nu}q$$

You may recognize these operators...

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The quantities of interest can be determined by making use of the Feynman-Hellman Theorem and simple spectroscopic LQCD calculations

$$\Delta_q M_N = \tilde{c}_0 \frac{\partial M_N[\tilde{c}_0\mathcal{O}_0]}{\partial\tilde{c}_0} \qquad \delta_q M_N = \tilde{c}_3 \frac{\partial M_N[\tilde{c}_c\mathcal{O}_3]}{\partial\tilde{c}_3}$$

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We also need to determine

$$\sigma_{\pi N} = m_l \frac{\partial M_N}{\partial m_l} \qquad \delta M_N = \delta \frac{\partial M_N}{\partial\delta}$$

$$m_l = \frac{m_d + m_u}{2} \qquad \delta = \frac{m_d - m_u}{2}$$

Computational Strategy

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Simple spectroscopic LQCD calculations can be used to determine these important long-range CP-Violating pion-nucleon couplings

Spectroscopic calculations are what we are best at

Computational Strategy

- Quark Chromo-EDM Operators

$$\mathcal{O}_0 = -\frac{1}{2}\bar{q}\sigma_{\mu\nu}G^{\mu\nu}q \qquad \mathcal{O}_3 = -\frac{1}{2}\bar{q}\tau_3\sigma_{\mu\nu}G^{\mu\nu}q$$

  The leading contribution will come from the valence quarks (experience with valence/sea quark mass contribution to nucleon mass) - begin with this contribution

- Invert the valence quarks with a modified Dirac operator

$$D_\lambda = D + \lambda\{\mathcal{O}_0, \mathcal{O}_3\}$$

- Construct nucleon correlation function with these quarks and determine the resulting nucleon mass

- Vary λ and determine slope of mass correction to get derivative

$$\Delta_q M_N = \tilde{c}_0 \frac{\partial M_N[\tilde{c}_0\mathcal{O}_0]}{\partial \tilde{c}_0} \qquad \delta_q M_N = \tilde{c}_3 \frac{\partial M_N[\tilde{c}_c\mathcal{O}_3]}{\partial \tilde{c}_3}$$

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A new method for computing quark bi-linear matrix elements

developed with Chris Bouchard & Kostas Orginos
software development also from Thorsten Kurth

Feynman-Hellman Theorem

The Feynman-Hellman Theorem (FHT) relates matrix elements to (variations in) the spectrum

$$\frac{\partial E_n}{\partial \lambda} = \langle n | H_\lambda | n \rangle$$

The FHT is often used to determine the scalar quark matrix elements in the nucleon (needed to interpret direct dark matter detection) both with Chiral Perturbation Theory and direct lattice QCD calculations

$$m_q \frac{\partial m_N}{\partial m_q}\bigg|_{m_q = m_q^{\mathrm{phy}}} = \langle N | m_q \bar{q} q | N \rangle$$

Feynman-Hellman Theorem and Matrix Elements

Can the FHT be used to compute other matrix elements?

Yes! By now, it has been implemented by
CSSM + QCDSF/UKQCD, PRD90 (2014) [1405.3019]
to explore nucleon structure

I will describe an improved implementation and also relate the method to another popular newly revived method of computing matrix elements - the “summation method”

Feynman-Hellman Theorem and Matrix Elements

Consider a two point correlation function in the presence of some source

$$C_\lambda(t) = \langle\lambda|\hat{O}(t)\hat{O}^\dagger(0)|\lambda\rangle$$
$$= \frac{1}{\mathcal{Z}_\lambda}\int D\Phi e^{-S-S_\lambda} O(t)O^\dagger(0)$$

$$|\lambda\rangle \equiv \lambda\text{-vacuum}$$
$$|\Omega\rangle \equiv \lim_{\lambda\to 0}|\lambda\rangle$$

$$S_\lambda = \lambda\int d^4x j(x)$$

$$j(x) = \text{ some bi-linear current density}$$

$$\text{e.g. } \lambda j(x) = \bar{q}(x) m_q q(x)$$

Feynman-Hellman Theorem and Matrix Elements

We can differentiate the correlator with respect to **λ**

$$-\frac{\partial C_\lambda}{\partial \lambda} = \frac{\partial_\lambda \mathcal{Z}_\lambda}{\mathcal{Z}_\lambda} C_\lambda(t) + \frac{1}{\mathcal{Z}_\lambda} \int D\Phi e^{-S-S_\lambda} \int d^4x' j(x')\ \mathcal{O}(t)\mathcal{O}^\dagger(0)$$

The first term is proportional to a vacuum matrix element and the second contains the matrix element we are interested in. We are really interested in the linear-response

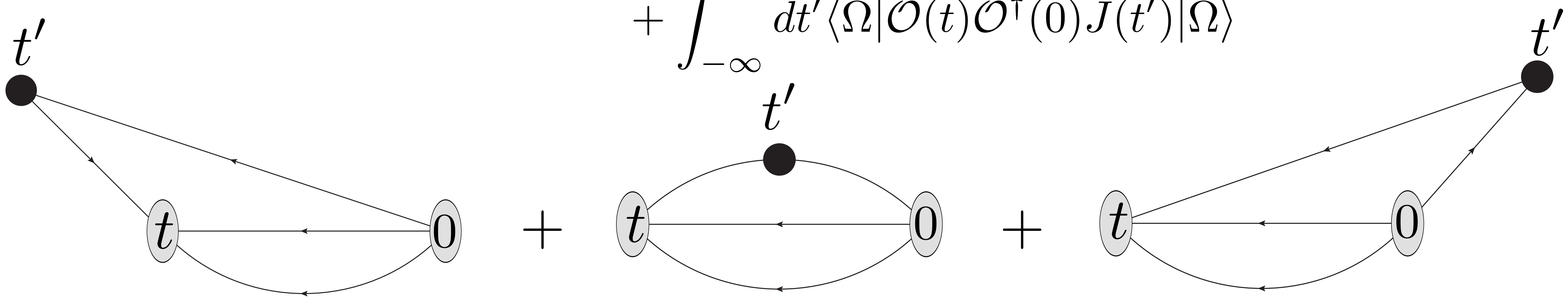
$$-\frac{\partial C_\lambda(t)}{\partial \lambda}\bigg|_{\lambda=0} = -C_\lambda(t) \int d^4x' \langle \Omega | j(x') | \Omega \rangle + \int dt' \langle \Omega | T\{\mathcal{O}(t) J(t') \mathcal{O}^\dagger(0)\} | \Omega \rangle$$

$$J(t) = \int d^3x\ j(t, \mathbf{x})$$

Feynman-Hellman Theorem and Matrix Elements

Let us focus on the second term:

$$\int dt' \langle\Omega|T\{\mathcal{O}(t)J(t')\mathcal{O}^\dagger(0)\}|\Omega\rangle = \int_t^\infty dt' \langle\Omega|J(t')\mathcal{O}(t)\mathcal{O}^\dagger(0)|\Omega\rangle + \int_0^t dt' \langle\Omega|\mathcal{O}(t)J(t')\mathcal{O}^\dagger(0)|\Omega\rangle + \int_{-\infty}^t dt' \langle\Omega|\mathcal{O}(t)\mathcal{O}^\dagger(0)J(t')|\Omega\rangle$$



(+ disconnected pieces)

The middle contribution is in fact similar to the summation method, summed over all time slices between the source and sink

Feynman-Hellman Theorem and Matrix Elements

The FHT relates matrix elements to the spectrum. Can we find something similar in QFT?

Let us try the first obvious thing, take a derivative of the effective mass:

$$m^{eff}(t,\tau) = \frac{1}{\tau}\ln\left(\frac{C(t)}{C(t+\tau)}\right) \underset{t\to\infty}{\longrightarrow} \frac{1}{\tau}\ln(e^{E_0\tau})$$

$$\left.\frac{\partial m_\lambda^{eff}(t,\tau)}{\partial\lambda}\right|_{\lambda=0} = \frac{1}{\tau}\left[\frac{-\partial_\lambda C_\lambda(t+\tau)}{C(t+\tau)} - \frac{-\partial_\lambda C_\lambda(t)}{C(t)}\right]$$

NOTE: even for currents with non-vanishing vacuum matrix elements, this contribution exactly cancels in this quantity

Feynman-Hellman Theorem and Matrix Elements

We are then left with the following

$$\partial_\lambda m_\lambda^{eff}(t,\tau)\Big|_{\lambda=0} = \frac{R(t+\tau)-R(t)}{\tau}$$

$$R(t) = \frac{\int dt' \langle 0|T\{\mathcal{O}(t)J(t')\mathcal{O}(0)\}|0\rangle}{C(t)}$$

To understand this quantity, we begin by inserting complete set's of states where appropriate

$$\begin{aligned} C(t) &= \langle\Omega|\mathcal{O}(t)\mathcal{O}^\dagger(0)|\Omega\rangle \\ &= \sum_n \langle\Omega|e^{\hat{H}t}\mathcal{O}(0)e^{-\hat{H}t}\frac{|n\rangle\langle n|}{2E_n}\mathcal{O}^\dagger(0)|\Omega\rangle \\ &= \sum_n Z_n Z_n^\dagger \frac{e^{-E_n t}}{2E_n} \end{aligned}$$

$$Z_n \equiv \langle\Omega|\mathcal{O}|n\rangle$$

$$Z_n^\dagger \equiv \langle n|\mathcal{O}^\dagger|\Omega\rangle$$

Feynman-Hellman Theorem and Matrix Elements

The numerator term we can separate into the three regions:

$$t' < 0, \quad 0 \leq t' \leq t, \quad t < t'$$

I II III

The middle region, II, is the region we are interested in, where we have the matrix element of interest. The other two regions will contribute to systematics that must be controlled.

Feynman-Hellman Theorem and Matrix Elements

After some algebra and finite sums, one finds for region II:

$$\frac{\sum_{t'=0}^{t}\langle\Omega|\mathcal{O}(t)J(t')\mathcal{O}(0)|\Omega\rangle}{\frac{Z_0 Z_0^\dagger e^{-E_0 t}}{2E_0}} = t\frac{\langle 0|J|0\rangle}{2E_0}\left(1+\sum_{n>0}\frac{Z_n Z_n^\dagger}{Z_0 Z_0^\dagger}\frac{E_0^2}{E_n^2}e^{-\Delta_{n0}t}\frac{\langle n|J|n\rangle}{\langle 0|J|0\rangle}\right)$$
$$+\sum_{n>0}\frac{1}{2E_n}\frac{1-e^{-\Delta_{n0}(t+1)}}{1-e^{-\Delta_{n0}}}\left(\frac{Z_n^\dagger}{Z_0^\dagger}\langle 0|J|n\rangle+\frac{Z_n}{Z_0}\langle n|J|0\rangle\right)$$
$$+\sum_{n>0,m\neq\{0,n\}}\frac{Z_n Z_m^\dagger}{Z_0 Z_0^\dagger}\frac{E_0}{2E_n E_m}\frac{1-e^{-\Delta_{nm}(t+1)}}{1-e^{-\Delta_{nm}}}\langle n|J|m\rangle$$

$$\Delta_{nm}\equiv E_n - E_m$$

NOTE: the term we are interested in is enhanced by a factor of t

Feynman-Hellman Theorem and Matrix Elements

The contributions from regions I and III must have some symmetry. The easiest way to evaluate these terms is to consider a shifted coordinate system, and a symmetric correlation function about the origin

$$-\frac{T}{2} \leq t \leq \frac{T}{2}$$

I: $$\sum_{t'=-T/2}^{-t/2-1} \langle \Omega | \mathcal{O}(t/2) \mathcal{O}^\dagger(-t/2) J(t') | \Omega \rangle$$

II: $$\sum_{t'=t/2+1}^{T/2} \langle \Omega | J(t') \mathcal{O}(t/2) \mathcal{O}^\dagger(-t/2) | \Omega \rangle$$

It is straightforward to show this is equivalent to summing over just the first lattice and non of it's images

Feynman-Hellman Theorem and Matrix Elements

The sum to the matrix element from these two regions is

$$\frac{\left[\sum_{t'=-T/2}^{-t/2-1} + \sum_{t'=t/2+1}^{T/2}\right] \langle\Omega|\mathcal{O}(t/2)J(t')\mathcal{O}^\dagger(-t/2)|\Omega\rangle}{\frac{Z_0 Z_0^\dagger e^{-E_0 t}}{2E_0}}$$

$$= \sum_{n,m_J} e^{-\Delta_{n0}t}\frac{E_0}{2E_n E_{m_J}}\frac{1-e^{-E_{m_J}(T/2-t/2)}}{e^{E_{m_J}}-1}\left(\frac{Z_n Z_{nm_J}^\dagger}{Z_0 Z_0^\dagger}\langle m_J|J|\Omega\rangle + \frac{Z_n^\dagger Z_{m_J n}}{Z_0 Z_0^\dagger}\langle\Omega|J|m_J\rangle\right)$$

$$E_{m_J} = \text{(mesonic) states which couple to the current, J}$$

$$\langle m_J|J|\Omega\rangle$$

$$Z_{nm_J} \equiv \langle n|\mathcal{O}|m_J\rangle$$

These terms are also not enhanced by t

Feynman-Hellman Theorem and Matrix Elements

The expression for R(t) is not obviously useful. The "magic" happens when we consider the differentiation of the effective mass

$$\partial_\lambda m_\lambda^{eff}(t,\tau)\Big|_{\lambda=0} = \frac{R(t+\tau) - R(t)}{\tau}$$

What we are left with in the end, is an expression of the form (for fixed τ)

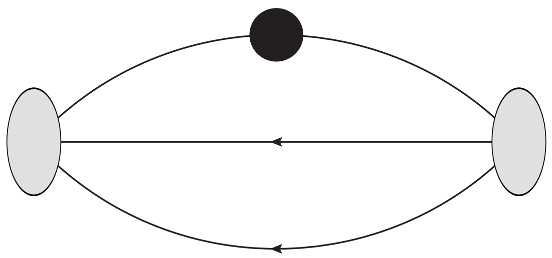
$$\partial_\lambda m_\lambda^{eff}(t,\tau)\Big|_{\lambda=0} = \frac{\langle 0|J|0\rangle}{2E_0} + (Ct + D)e^{-\Delta t}$$

There are no time-independent contributions other than the matrix element of interest

Practical Implementation:

We are interested in the linear response of the theory to external sources.

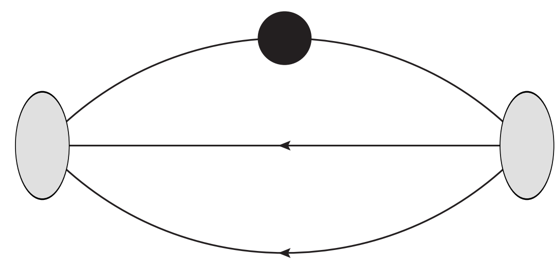
At the level of a QCD correlation function, we are then interested in only a single insertion of the current on the quark propagator, such that the proton for example, would have a contribution



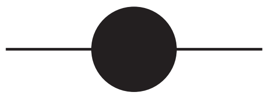
One then makes suitable replacements of all the quark flavor-lines with the "Feynman-Hellman" propagator

Feynman-Hellman Theorem and Matrix Elements

Practical Implementation:



the "Feynman-Hellman" propagator is given by



$$= S_{FH}(y,x) = \sum_z S(y,z)\Gamma(z)S(z,x)$$

$S(z,x)$ standard quark propagator off some source at x, to all z

$\Gamma(z)$ some bi-linear operator (can be constant)
e.g., γ_4 for the vector current

$\Gamma(z)S(z,x)$ treat like a source to invert off of

Feynman-Hellman Theorem and Matrix Elements

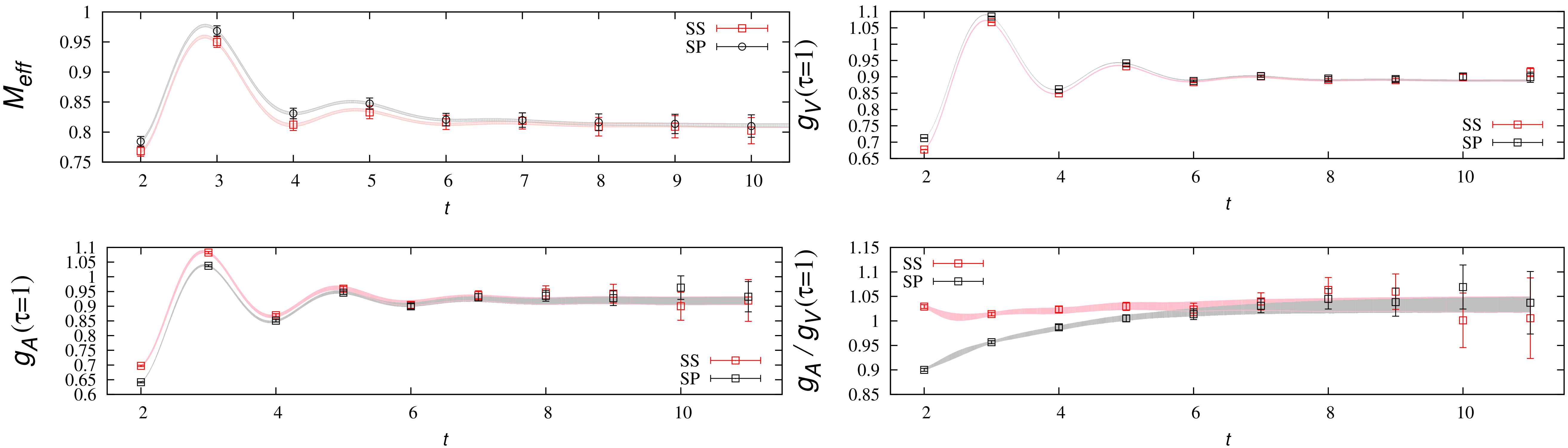
Test case: nucleon axial charge, LHPC comparison

there are old LHPC calculations of the nucleon axial charge with moderate pion masses using DWF on asqtad MILC ensembles

the “regular” propagators were on disk at JLab, so we could simply make the Feynman-Hellman propagators

Feynman-Hellman Theorem and Matrix Elements

Test case: nucleon axial charge, LHPC comparison



our results are in exquisite agreement with LHPC PRD 82 (2010), arXiv:1001.3620

(the oscillations are from a large domain wall mass, $M_5 = 1.7$)

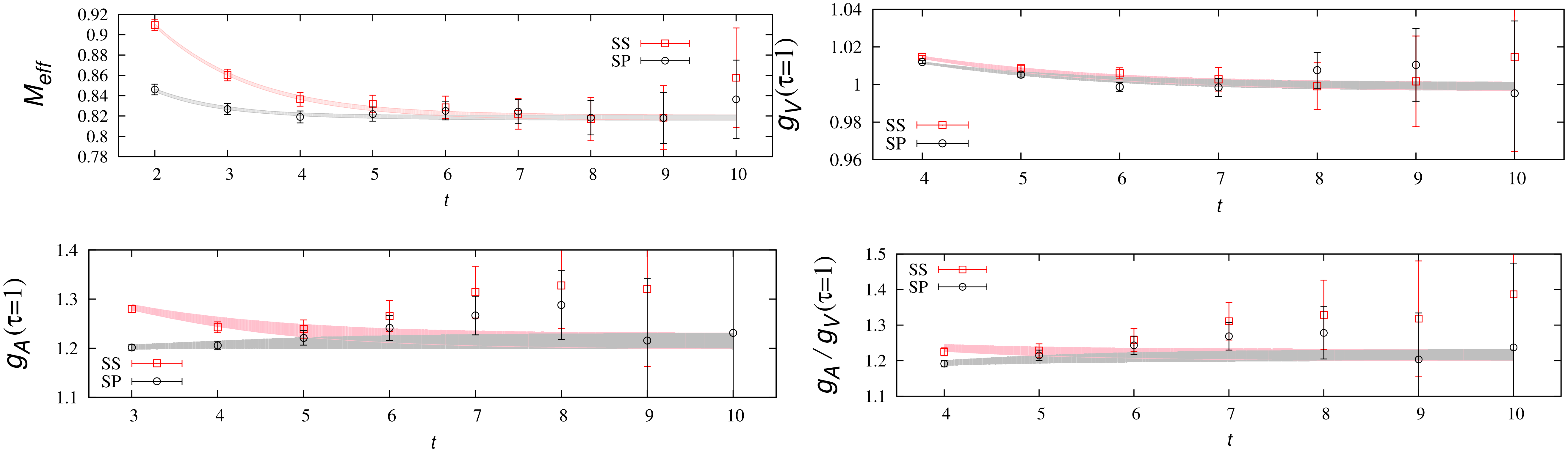
Feynman-Hellman Theorem and Matrix Elements

Test case: nucleon axial charge, DWF on HISQ

$$m_\pi \simeq 310 \text{ MeV}$$

$$a \simeq 0.15 \text{ fm}$$

we are doing our quark CEDM calculation with this setup



Feynman-Hellman Theorem and Matrix Elements

This is equivalent to taking functional derivatives of the partition function with respect to the perturbing source, then setting the source to zero.

It can be applied to non-zero matrix elements

It can be applied to flavor changing matrix elements

…

Conclusions

This is an exciting time for low-energy precision tests of the Standard Model.

Lattice QCD is an essential aspect of this research field as it is the only non-perturbative regulator of QCD, and therefore it allows us to quantitatively understand the manifestation/interactions of BSM physics within nuclear environments.