Multi-nucleon Matrix Elements on the Lattice with E-graph Optimised Wick Contractions and the Feynman-Hellmann Theorem

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Nuclear Structure Through Lattice QCD

- This work seeks to enable and explore more detailed lattice probes into the nuclear structure of (relatively) large nuclei
- Let A denote the number of nucleons in a nuclei state $|X\rangle$
- Explore multi-nucleon lattice probes using the Forward Compton Tensor as an example
- Key Challenges:
  1. Signal-to-Noise scaling: errors generally scale poorly with quark number
  2. Identifying physically relevant states: achieving good overlap with the ground-state becomes increasingly difficult for many-hadron systems
  3. Numerical correlator evaluation:
     - Wick contractions scale factorially in quark number
     - Index set scales exponentially in quark number
     - Floating point errors interact poorly with delicate cancellations

Tensor E-graphs

PRELIMINARY

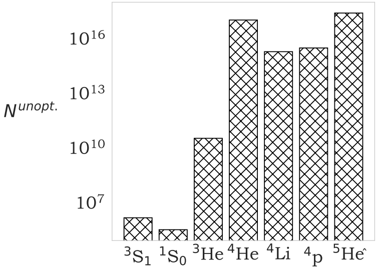


Figure 1: The number of operations ($N^{unopt.}$) required to directly evaluate the correlator expressions via the hadron block method, excluding the number of operations required to evaluate the single nucleon blocks themselves.

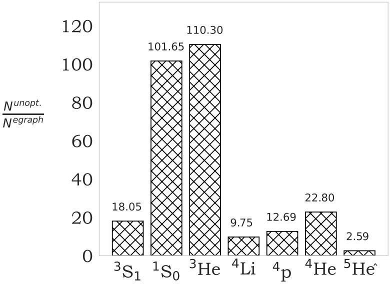
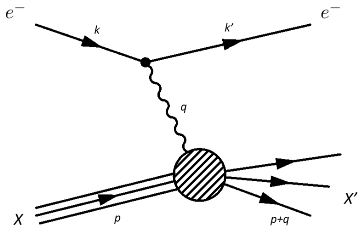


Figure 2: Performance of the tensor e-graph method for nuclear correlation functions for the deuteron ($^3S_1$), dinueutron ($^1S_0$), helium-3 (^3He), and helium-4 (^4He), lithium-4 (^4Li), four proton (^4p), and helium-5 ($^5\hat{He}$) operators.

arXiv:2201.04269 [hep-lat]

DIS and Kinematics



- Typically X = baryon, but this work sets X = multi-hadron state
- k (k') incoming (outgoing) lepton momenta
- p incoming momentum of X state
- $d\sigma \sim L^{\mu\nu} W_{\mu\nu}$ scales as lepton tensor $L^{\mu\nu}$ and hadron tensor $W^{\mu\nu}$.

$$W_{\mu\nu}(p,q) = \left(-g_{\mu\nu} + \frac{q_\mu q_\nu}{q^2}\right) F_1(x,Q^2) + \left(p_\mu - \frac{p\cdot q}{q^2} q_\mu\right)\left(p_\nu - \frac{p\cdot q}{q^2} q_\nu\right) \frac{F_2(x,Q^2)}{p\cdot q} \tag{1}$$

$$x := \frac{Q^2}{2p\cdot q} \quad \text{Bjorken scaling variable,} \quad Q^2 = -q^2 \tag{2}$$

Observables

Forward (unpolarised) Compton Tensor:

$$T_{\mu\nu}(p,q) := i \int d^4 z e^{i\vec{q}\cdot\vec{z}} \rho_{ss'} \langle X'_{p,s'} | \mathcal{T}\{\mathcal{J}_\mu(z)\mathcal{J}_\nu(0)\} | X_{p,s} \rangle \tag{3}$$

$$=: \left(-g_{\mu\nu} + \frac{q_\mu q_\nu}{q^2}\right)\mathcal{F}_1(\omega, Q^2) + \left(p_\mu - \frac{p\cdot q}{q^2} q_\mu\right)\left(p_\nu - \frac{p\cdot q}{q^2} q_\nu\right)\frac{\mathcal{F}_2(\omega, Q^2)}{p\cdot q} \tag{4}$$

where:

$$\omega := \frac{2p\cdot q}{Q^2} = \frac{1}{x} \qquad \text{Inverse Bjorken scaling variable} \tag{5}$$

$$\mathcal{J}_\mu(z) = Z_V \bar{q}(z)\gamma_\mu q(z) \tag{6}$$

Can resolve Compton Structure Functions (in Minkowski space):

$$\mathcal{F}_1(w, Q^2) = T_{33}(p,q) \tag{7}$$

$$\frac{\mathcal{F}_2(w, Q^2)}{\omega} = \frac{Q^2}{2E_X^2}\left[T_{00}(p,q) + T_{33}(p,q)\right] \tag{8}$$

Feynman-Hellmann

$$\frac{T_{\mu\mu}(p,q) + T_{\mu\mu}(p,-q)}{2} = -E_X(\vec{p})\frac{\partial^2 E_{X_\lambda}}{\partial \lambda^2}\bigg|_{\lambda=0} \tag{9}$$

where $E_{X,\lambda}$:

$$C_\lambda(\vec{p};t,q) := \int d^3\vec{z} e^{-i\vec{p}\cdot\vec{z}} \langle \Omega_\lambda | X(\vec{z};t)\overline{X}(0) |\Omega_\lambda\rangle \tag{10}$$

$$\simeq A_\lambda e^{-E_{X,\lambda} t} \tag{11}$$

where $|\Omega_\lambda\rangle$ is obtained via a perturbation to the fermion action:

$$S(\lambda) = S_{unpert} + \lambda \int d^4 z \left(e^{iq\cdot z} + e^{-iq\cdot z}\right) \mathcal{J}_\mu(z) \tag{12}$$

See other QCHSC24 FH contributions:

- James **Zanotti** [Constraining beyond the Standard Model nucleon isovector charges]
- K. Utku **Can** [The parity-odd structure function of the nucleon from the Compton amplitude in lattice QCD]
- Jordan **McKee** [Compton Amplitude of the Pion using Feynman-Hellmann]
- Thomas **Schar** [Reduction of discretisation artifacts in the lattice subtraction function calculation]
- Ian **van Schalkwyk** [Calculation of the Compton Amplitude at High Momentum using Momentum Smearing]

Proton Target Results

$$\frac{\mathcal{F}_2(w, Q^2)}{\omega} = \frac{Q^2}{2E_p^2}\left[T_{00}(p,q) + T_{33}(p,q)\right]$$

$$\mathcal{F}_2(\omega, Q^2) = \sum_{n=1}^{\infty} 4\omega^{2n-1} M_{2n}^{(2)}(Q^2)$$

- Q^2 fit dependence:

$$M_{2,h}^{(2)}(Q^2) = M_{2,h}^{(2)} + \frac{C_{2,h}^{(2)}}{Q^2} + \mathcal{O}(1/Q^4)$$

- Moment construction:

$$M_{2,p}^{(2,L)} = \frac{4}{9} M_{2,uu}^{(2,L)} + \frac{1}{9} M_{2,dd}^{(2,L)} - \frac{2}{9} M_{2,ud}^{(2,L)}$$

where $h \in \{uu, dd, ud, p\}$

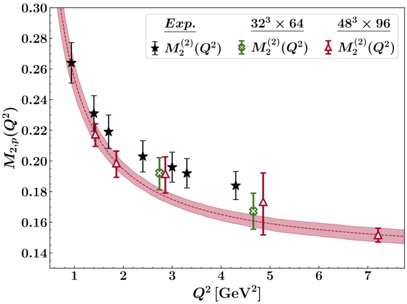


Figure 3: Q^2 dependence of the lowest moments of $\mathcal{F}_2$ for the proton. Filled stars are the experimental Cornwall-Norton moments of $\mathcal{F}_2$ taken from Table I of Ref. [PRD 63.094008]. We have assigned a 5% error to the experimental moments as indicated in Ref. [PRD 63.094008]. Red band is the fit to the 48 × 96 data points.

[Phys.Rev.D 107 (2023) 5, 054503]

Proton Target Results

$$\frac{\mathcal{F}_2(w,Q^2)}{\omega} = \frac{Q^2}{2E_p^2}\left[T_{00}(p,q) + T_{33}(p,q)\right]$$

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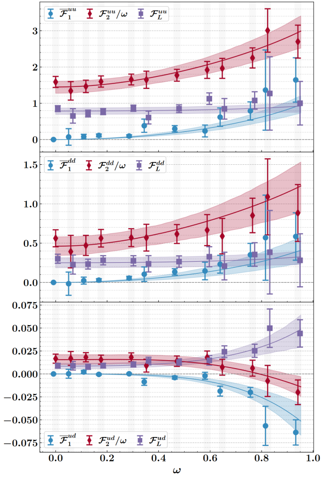
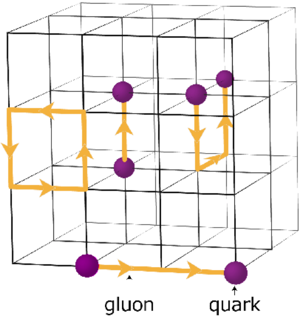


[Phys.Rev.D 107 (2023) 5, 054503]

Lattice QCD Details

- QCDSF $32^3 \times 64$ configurations with 2+1 flavour
- NP-improved Clover action with $\beta = 5.50$
- $\sim SU(3)$ symmetric point
- Lattice space $a = 0.074$ fm
- $m_\pi \sim 470$ MeV
- $m_\pi L \sim 5.6$
- $\lambda \in \{\pm\lambda_1, \pm\lambda_2\}$ where $\lambda_1 = 0.025$, $\lambda_2 = 0.05$
- Purely connected contributions
- Low-statistics exploratory results (for everything herein):
  - $n_{src} \sim 1$
  - $n_{confs} \sim 1200$



Operators and Correlated Ratios

Local interpolating operators:

$$p^{\pm}_{\alpha}(x) = \epsilon^{abc}\left[[u^{a}(x)]^{T}(C\gamma_5 P_{\pm})d^{b}(x)\right]u^{c}_{\alpha}(x) \tag{13}$$

$$n^{\pm}_{\alpha}(x) = \epsilon^{abc}\left[[d^{a}(x)]^{T}(C\gamma_5 P_{\pm})u^{b}(x)\right]d^{c}_{\alpha}(x), \tag{14}$$

where $P_{\pm} = \frac{1}{2}(1 \pm \gamma_4)$.

$NN(^3S_1)$ Deuteron with $J^P = 1^+$, $J_z = +1$:

$$\mathscr{O}_{^3S_1}(x) = \frac{1}{\sqrt{2}}\left(\left[p^{+}(x)\right]^{T}(C\gamma_3)n^{+}(x) - \left[n^{+}(x)\right]^{T}(C\gamma_3)p^{+}(x)\right) \tag{15}$$

Perturbed Ratio:

$$R^{(\lambda)}(t) = \frac{\langle C_{\lambda}(t)\rangle\langle C_{-\lambda}(t)\rangle}{[\langle C_{\lambda=0}(t)\rangle]^2} \tag{16}$$

$$\sim A_{\lambda}e^{-2\Delta E_X t} \tag{17}$$

Deuteron Quark Counting

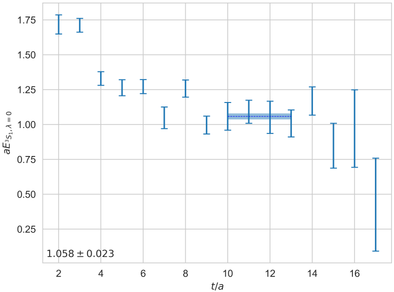
- Before getting to:
  $T_{\mu\nu}(p,q) = i\int d^4 z e^{i\vec{q}\cdot\vec{z}} \rho_{ss'} \langle X'_{p,s'} | \mathcal{T}\{\mathcal{J}_\mu(z)\mathcal{J}_\nu(0)\} | X_{p,s}\rangle$
  Calculate $\vec{q} = \vec{0} = \vec{p}$ single current insertion object:

$$\mathcal{O} = \int d^4 z \, \langle \mathcal{O}_{^3S_1} | \mathcal{J}_{\mu=4}(z) | \mathcal{O}_{^3S_1} \rangle$$

- Nucleon g.s. reference energy scale $aE_{nuc,\lambda=0} = 0.50(8)$
- Perturbation applied to all up quark propagators, so expect:

$$aZ_V \frac{\partial E_{^3S_1}}{\partial \lambda}\bigg|_{\lambda=0} = 3$$

Unperturbed $NN(^3S_1)$ Effective Energy Fit



$$aE_{^3S_1,\lambda=0} = 1.06 \pm 0.02$$

Deuteron Quark Counting

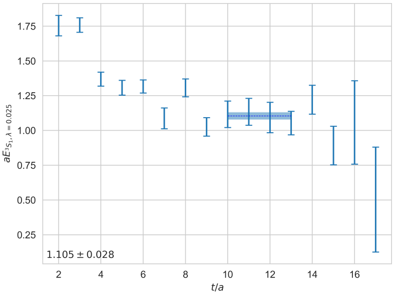
- Before getting to:
  $T_{\mu\nu}(p,q) = i\int d^4 z e^{i\vec{q}\cdot\vec{z}} \rho_{ss'} \langle X'_{p,s'} | \mathcal{T}\{\mathcal{J}_\mu(z)\mathcal{J}_\nu(0)\} | X_{p,s} \rangle$
  Calculate $\vec{q} = \vec{0} = \vec{p}$ single current insertion object:

$$\mathcal{O} = \int d^4 z \, \langle \mathcal{O}_{^3S_1} | \mathcal{J}_{\mu=4}(z) | \mathcal{O}_{^3S_1} \rangle$$

- Nucleon g.s. reference energy scale $aE_{nuc,\lambda=0} = 0.50(8)$
- Perturbation applied to all up quark propagators, so expect:

$$aZ_V \frac{\partial E_{^3S_1}}{\partial \lambda}\bigg|_{\lambda=0} = 3$$

Perturbed $NN(^3S_1)$ Effective Energy Fit at $\lambda = \lambda_1 = 0.025$



$$aE_{^3S_1,\lambda=\lambda_1} = 1.11 \pm 0.03$$

Deuteron Quark Counting

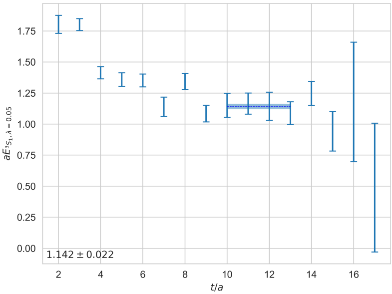
- Before getting to:
  $T_{\mu\nu}(p,q) = i\int d^4z e^{i\vec{q}\cdot\vec{z}}\rho_{ss'}\langle X'_{p,s'}|\mathcal{T}\{\mathcal{J}_\mu(z)\mathcal{J}_\nu(0)\}|X_{p,s}\rangle$
  Calculate $\vec{q}=\vec{0}=\vec{p}$ single current insertion object:

$$\mathcal{O} = \int d^4z \langle \mathcal{O}_{^3S_1}|\mathcal{J}_{\mu=4}(z)|\mathcal{O}_{^3S_1}\rangle$$

- Nucleon g.s. reference energy scale $aE_{nuc,\lambda=0} = 0.50(8)$
- Perturbation applied to all up quark propagators, so expect:

$$aZ_V \frac{\partial E_{^3S_1}}{\partial\lambda}\bigg|_{\lambda=0} = 3$$

Perturbed $NN(^3S_1)$ Effective Energy Fit at $\lambda = \lambda_2 = 0.05$



$$aE_{^3S_1,\lambda=\lambda_2} = 1.14 \pm 0.02$$

Deuteron Quark Counting

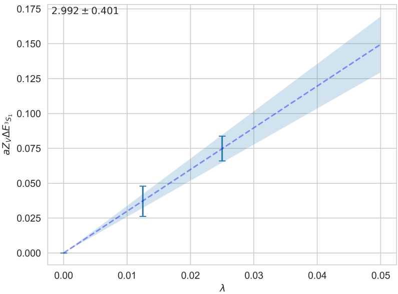
- Before getting to:
  $T_{\mu\nu}(p,q) = i\int d^4 z e^{i\vec{q}\cdot\vec{z}} \rho_{ss'} \langle X'_{p,s'} | \mathcal{T}\{\mathcal{J}_\mu(z)\mathcal{J}_\nu(0)\} | X_{p,s}\rangle$
  Calculate $\vec{q} = \vec{0} = \vec{p}$ single current insertion object:

$$\mathcal{O} = \int d^4 z \, \langle \mathcal{O}_{^3S_1} | \mathcal{J}_{\mu=4}(z) | \mathcal{O}_{^3S_1} \rangle$$

- Nucleon g.s. reference energy scale $aE_{nuc,\lambda=0} = 0.50(8)$
- Perturbation applied to all up quark propagators, so expect:

$$aZ_V \frac{\partial E_{^3S_1}}{\partial \lambda}\bigg|_{\lambda=0} = 3$$

$NN(^3S_1)$ Quark Counting Renormalised Lambda Fit



$$aZ_V \frac{\partial E_{^3S_1}}{\partial \lambda}\bigg|_{\lambda=0} = 2.992 \pm 0.4$$

T_{44} Results

PRELIMINARY

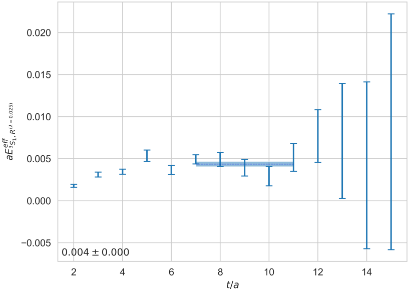
- Calculate:
  $T_{44}(p,q) = \int d^4 z e^{i\vec{q}\cdot\vec{z}} \langle {}^3S_1 | \mathcal{T}\{\mathcal{J}_4(z)\mathcal{J}_4(0)\} | {}^3S_1 \rangle$
- With:
  - $\vec{p} = 0$
  - $\vec{q} = (4,1,0)\frac{2\pi}{L}$, $Q^2 = 4.66\ \text{GeV}^2$
- Note Wick rotation: $T_{00} \to -T_{44}$
- Extracting ΔE_X via perturbed ratio:

$$R^{(\lambda)}(t) = \frac{\langle C_\lambda(t)\rangle\langle C_{-\lambda}(t)\rangle}{[\langle C_{\lambda=0}(t)\rangle]^2} \sim A_\lambda e^{-2\Delta E_X t}$$

- Calculate T_{44} via:
  $\frac{T_{\mu\mu}(p,q)+T_{\mu\mu}(p,-q)}{2} = -E_X(\vec{p})\frac{\partial^2 E_{X_\lambda}}{\partial\lambda^2}\Big|_{\lambda=0}$
- In terms of Forward Compton structure functions:

$$T_{44}(p,q) = \mathcal{F}_1(\omega, Q^2) - \frac{2E_X^2}{Q^2}\frac{\mathcal{F}_2(\omega,Q^2)}{\omega}$$

Perturbed $NN(^3S_1)$ Effective Energy Fit at $\lambda = \lambda_1 = 0.025$



$$aE_{^3S_1, R^{\lambda=\lambda_1}} = (4.3 \pm 0.3) \times 10^{-3}$$

T_{44} Results *PRELIMINARY*

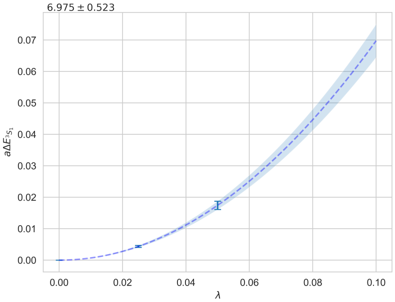
- Calculate:
  $T_{44}(p,q) = \int d^4 z e^{i\vec{q}\cdot\vec{z}} \langle {}^3S_1 | \mathcal{T}\{\mathcal{J}_4(z)\mathcal{J}_4(0)\} | {}^3S_1 \rangle$
- With:
  - $\vec{p} = 0$
  - $\vec{q} = (4,1,0)\frac{2\pi}{L}$, $Q^2 = 4.66$ GeV^2
- Note Wick rotation: $T_{00} \to -T_{44}$
- Extracting ΔE_X via perturbed ratio:

$$R^{(\lambda)}(t) = \frac{\langle C_\lambda(t)\rangle \langle C_{-\lambda}(t)\rangle}{[\langle C_{\lambda=0}(t)\rangle]^2} \sim A_\lambda e^{-2\Delta E_X t}$$

- Calculate T_{44} via:
  $\frac{T_{\mu\mu}(p,q)+T_{\mu\mu}(p,-q)}{2} = -E_X(\vec{p}) \frac{\partial^2 E_{X_\lambda}}{\partial\lambda^2}\Big|_{\lambda=0}$
- In terms of Forward Compton structure functions:

$$T_{44}(p,q) = \mathcal{F}_1(\omega, Q^2) - \frac{2E_X^2}{Q^2}\frac{\mathcal{F}_2(\omega,Q^2)}{\omega}$$

T_{44} $NN({}^3S_1)$ Lambda Fit



$$a\frac{\partial^2 E_{^3S_1}}{\partial\lambda^2}\Big|_{\lambda=0} = 6.98 \pm 0.52$$

$$T_{44} = -7.39 \pm 0.55$$

T_{33} Results *PRELIMINARY*

- Calculate:
  $T_{33}(p,q) = \int d^4 z e^{i\vec{q}\cdot\vec{z}} \langle {}^3S_1 | \mathcal{T}\{\mathcal{J}_3(z)\mathcal{J}_3(0)\} | {}^3S_1 \rangle$
- With:
  - $\vec{p} = 0$
  - $\vec{q} = (4,1,0)\frac{2\pi}{L},\ Q^2 = 4.66\ \mathrm{GeV}^2$
- Extracting ΔE_X via perturbed ratio:

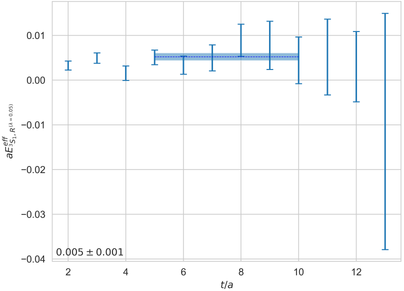
$$R^{(\lambda)}(t) = \frac{\langle C_\lambda(t)\rangle\langle C_{-\lambda}(t)\rangle}{[\langle C_{\lambda=0}(t)\rangle]^2} \sim A_\lambda e^{-2\Delta E_X t}$$

- Calculate T_{33} via:
  $\frac{T_{\mu\mu}(p,q)+T_{\mu\mu}(p,-q)}{2} = -E_X(\vec{p})\frac{\partial^2 E_{X_\lambda}}{\partial\lambda^2}\Big|_{\lambda=0}$
- Forward Compton structure functions:

$$\mathcal{F}_1(\omega, Q^2) = T_{33}(p,q)$$

$$\frac{\mathcal{F}_2(\omega, Q^2)}{\omega} = \frac{Q^2}{2E_X^2}\left[T_{33}(p,q) - T_{44}(p,q)\right]$$

Perturbed $NN({}^3S_1)$ Effective Energy Fit at $\lambda = \lambda_2 = 0.05$



$$aE_{^3S_1, R^{\lambda_2}} = (5.22 \pm 0.9) \times 10^{-3}$$

T_{33} Results PRELIMINARY

- Calculate:
  $T_{33}(p,q) = \int d^4 z e^{i\vec{q}\cdot\vec{z}} \langle {}^3S_1 | \mathcal{T}\{\mathcal{J}_3(z)\mathcal{J}_3(0)\} | {}^3S_1 \rangle$
- With:
  - $\vec{p} = 0$
  - $\vec{q} = (4,1,0)\frac{2\pi}{L}, \; Q^2 = 4.66 \text{ GeV}^2$
- Extracting ΔE_X via perturbed ratio:

$$R^{(\lambda)}(t) = \frac{\langle C_\lambda(t)\rangle\langle C_{-\lambda}(t)\rangle}{[\langle C_{\lambda=0}(t)\rangle]^2} \sim A_\lambda e^{-2\Delta E_X t}$$

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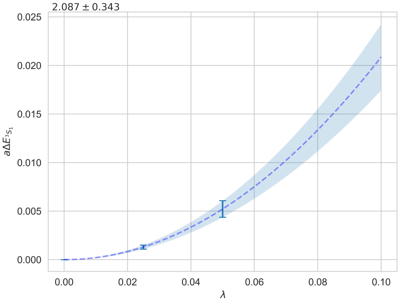
  $\frac{T_{\mu\mu}(p,q)+T_{\mu\mu}(p,-q)}{2} = -E_X(\vec{p})\frac{\partial^2 E_{X_\lambda}}{\partial\lambda^2}\Big|_{\lambda=0}$
- Forward Compton structure functions:

$$\mathcal{F}_1(\omega, Q^2) = T_{33}(p,q)$$

$$\frac{\mathcal{F}_2(\omega, Q^2)}{\omega} = \frac{Q^2}{2E_X^2}\left[T_{33}(p,q) - T_{44}(p,q)\right]$$

T_{33} $NN({}^3S_1)$ Lambda Fit



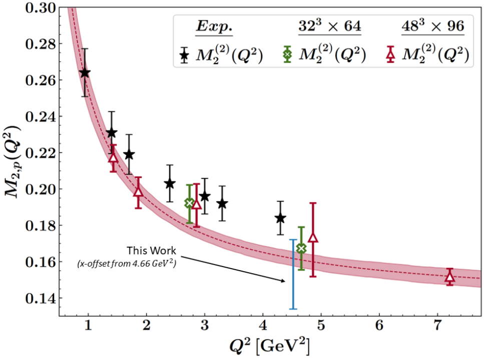
$$a\frac{\partial^2 E_{{}^3S_1}}{\partial\lambda^2}\Big|_{\lambda=0} = 2.09 \pm 0.34$$

$$\mathcal{F}_1 = T_{33} = -2.23 \pm 0.37$$

$$\frac{\mathcal{F}_2}{\omega} = 0.153 \pm 0.019$$

$M_2^{(2)}$ Result

PRELIMINARY



$$\frac{\mathcal{F}_2(w, Q^2)}{\omega} = \frac{Q^2}{2E_p^2}\left[T_{00}(p,q) + T_{33}(p,q)\right]$$

$$\mathcal{F}_2(\omega, Q^2) = \sum_{n=1}^{\infty} 4\omega^{2n-1} M_{2n}^{(2)}(Q^2)$$

$$M_{2,h}^{(2)}(Q^2) = M_{2,h}^{(2)} + \frac{C_{2,h}^{(2)}}{Q^2} + \mathcal{O}(1/Q^4)$$

$$M_{2,p}^{(2,L)} = \frac{4}{9} M_{2,uu}^{(2,L)} + \frac{1}{9} M_{2,dd}^{(2,L)} - \frac{2}{9} M_{2,ud}^{(2,L)}$$

Summary and Next Steps

Summary:

- Validated multi-nucleon FH process with quark counting exercise.
- Calculated $NN(^3S_1)$ $T_{33} = \mathcal{F}_1$ for $\vec{p} = \vec{0}$, $\vec{q} = (4, 1, 0)\frac{2\pi}{L}$, $Q^2 = 4.66 GeV^2$
- Calculated $NN(^3S_1)$ T_{44} and therefore $\mathcal{F}_2$ for $\vec{p} = \vec{0}$, $\vec{q} = (4, 1, 0)\frac{2\pi}{L}$, $Q^2 = 4.66 GeV^2$ to 12% precision
- Compared $NN(^3S_1)$ $\mathcal{F}_2$ lowest moment with proton results

Next Steps:

1. Repeat across a range of Q^2 values
2. Gather larger statistics
3. Improve $\mathcal{F}_2$ extraction mechanics
4. Increase A (e.g. helium-3, helium-4)
5. Multiple lattice parameters to establish dependence

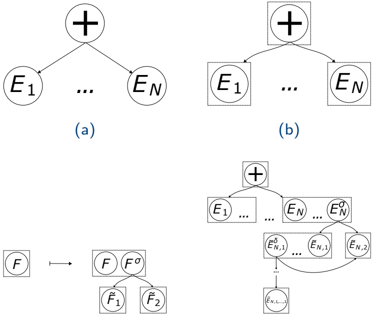


Figure 4: The evolution of a tensor e-graph, beginning with a directed acyclic graph representing the sum of N tensor expressions: $E_1 + \ldots + E_N$ (a), the introduction of e-classes (b), the application of the re-write rule (c), and the resultant tensor e-graph after construction (d).

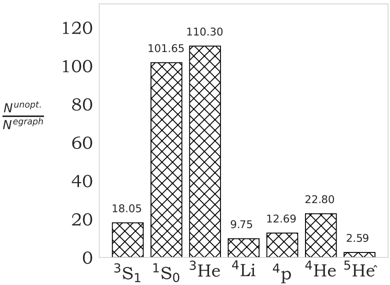


Figure 5: Performance of the tensor e-graph method for nuclear correlation functions for the deuteron ($^3S_1$), dinueutron ($^1S_0$), helium-3 (^3He), and helium-4 (^4He), lithium-4 (^4Li), four proton (^4p), and helium-5 ($^5\hat{He}$) operators.