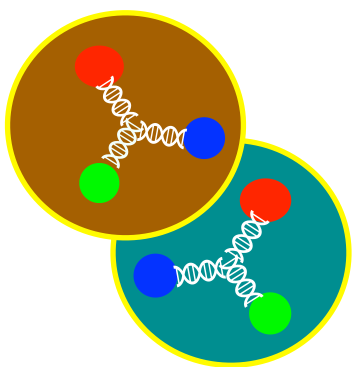
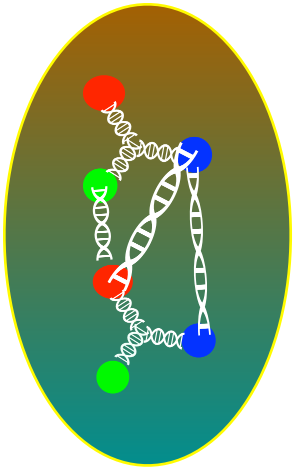
Few-Nucleon Systems in Lattice QCD





Michael Wagman

Brookhaven National Laboratory

High Energy / Nuclear Theory / RIKEN seminar

February 18, 2022

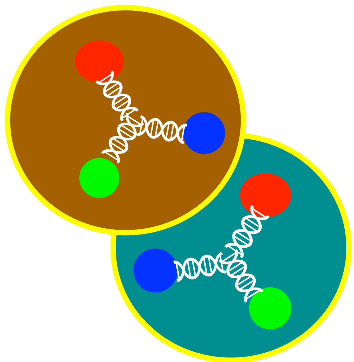
Fermilab

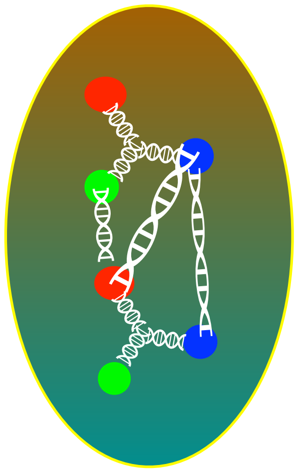
NPLQCD

Quarks, gluons, and nuclei

At low energies, nuclei “look like” collections of protons and neutrons

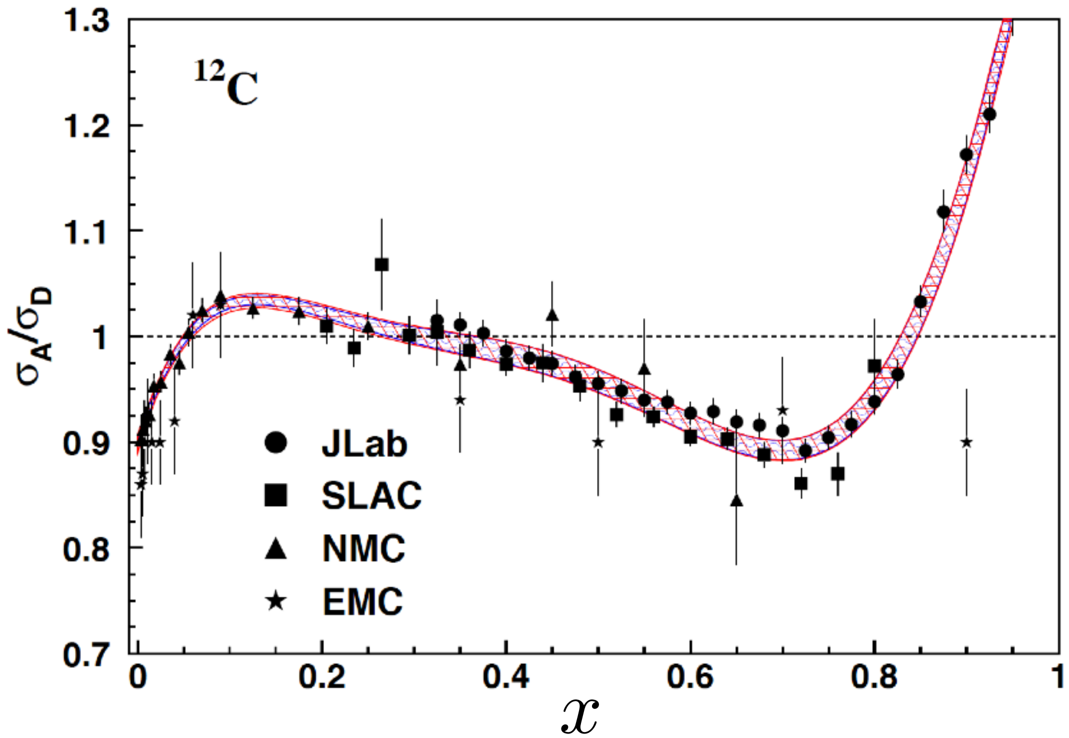
— Low-energy EFTs with nucleon degrees of freedom make accurate predictions





At high energies, nuclei “look like” collections of quarks and gluons

— Perturbative QCD makes accurate predictions for high-energy physics



Malace et al, Int. J. Mod. Phys. E 23 (2014)

Medium-energy interactions, as well as EFT input parameters and quark and gluon structure functions, contain rich nonperturbative physics

— Lattice QCD can provide accurate nonperturabtive predictions

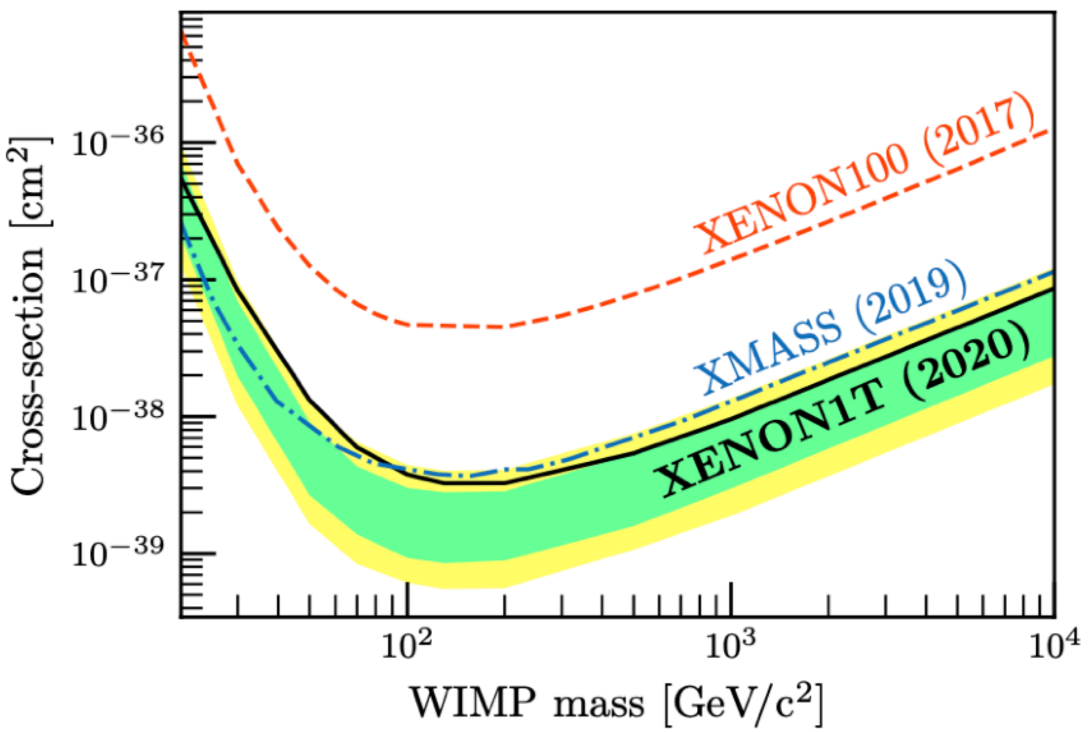
New physics and nuclei

Nuclei are useful experimental targets, cross-sections often grow with baryon number

Converting between nuclear- and nucleon-level cross-sections requires

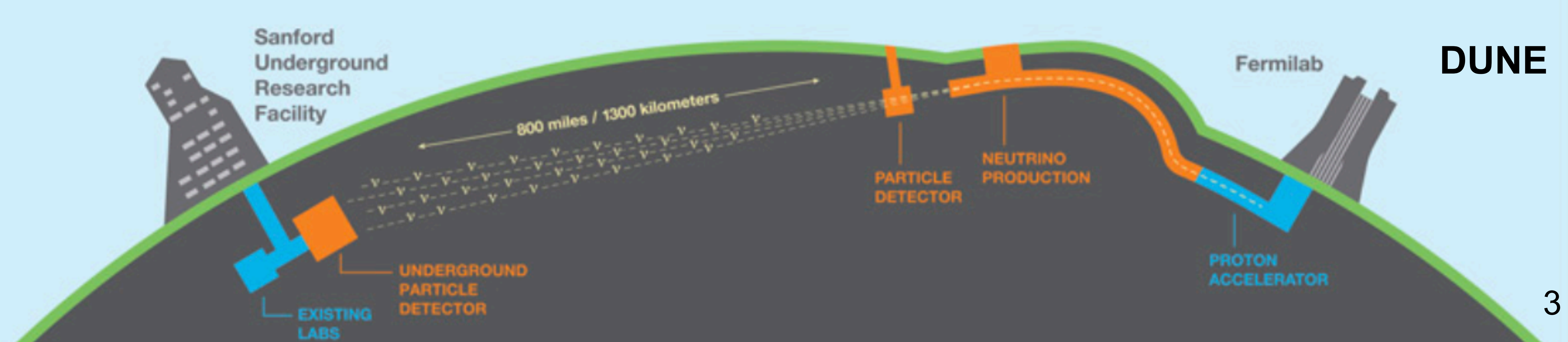
- Nuclear models (uncertainty quantification?)
- Direct LQCD calculations (impractical)
- LQCD informed EFT + modeling

Xenon1T constraint on dark matter-nucleus



Many low-energy searches for fundamental symmetry violation require nuclear matrix elements to relate experimental observables to new physics theory parameters

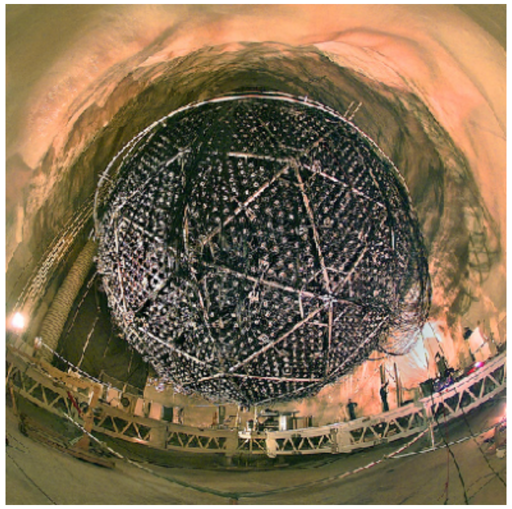
Standard Model predictions with controlled uncertainties essential for next-generation accelerator neutrino experiments aiming for few-percent systematic uncertainties



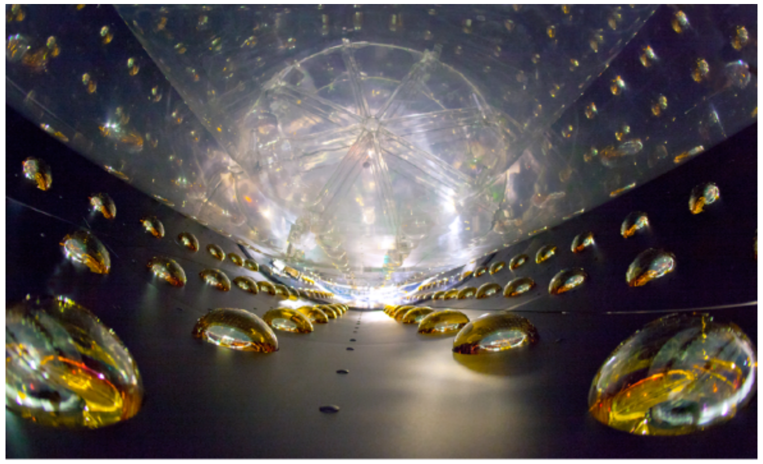
DUNE

Neutrino masses

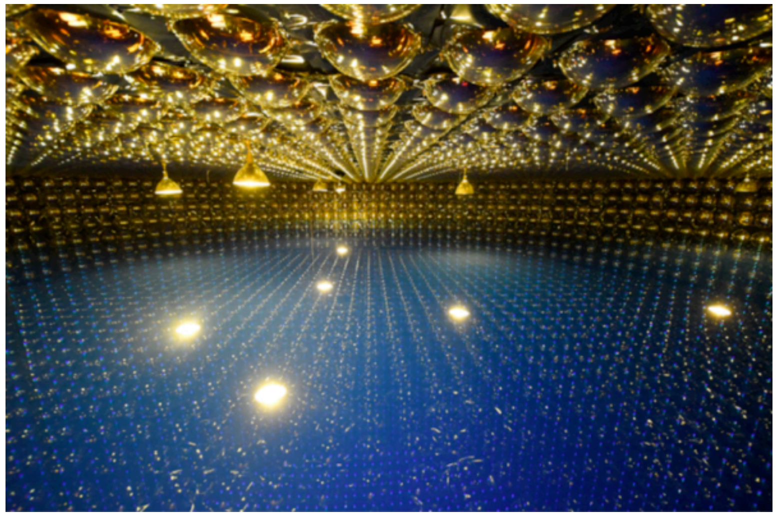
Experimentally observed neutrino oscillations require neutrinos to be massive



SNO



Daya Bay



Super K (K2K/T2K)

Solar, atmospheric, reactor, and accelerator neutrino experiments have constrained the 3 mixing angles in the PMNS matrix with few-percent precision

CP-violating phase is more poorly constrained

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = U_{PMNS} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3 \end{pmatrix}$$

Neutrino masses require physics beyond the Standard Model: right-handed sterile neutrinos and/or lepton-number-violating Majorana neutrino masses

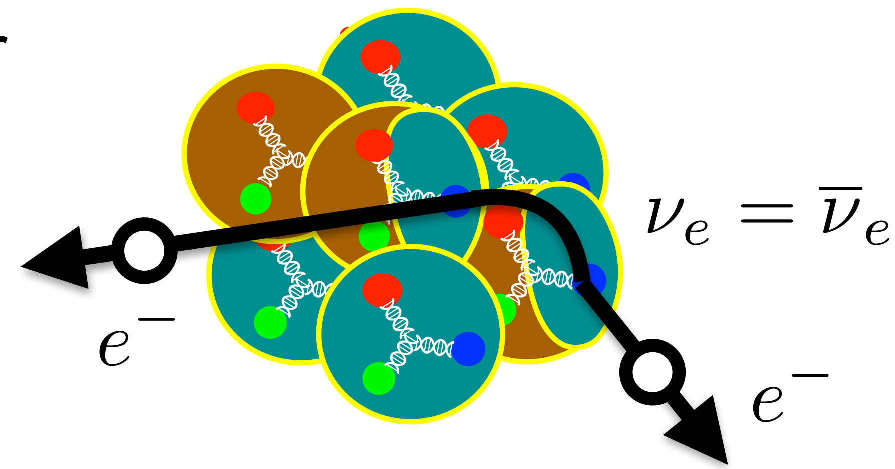
$$\mathcal{L}_5 \supset -\frac{1}{\Lambda}\varepsilon_{ab}(\overline{\ell}_{La}H_b)\varepsilon_{cd}(H_c^T C\overline{\ell}_{Ld}^T) + \text{h.c.} = -\frac{v^2}{\Lambda}(\overline{\nu}C\overline{\nu}^T + \nu^T C\nu) + \ldots$$

Weinberg, PRL 43 (1979)

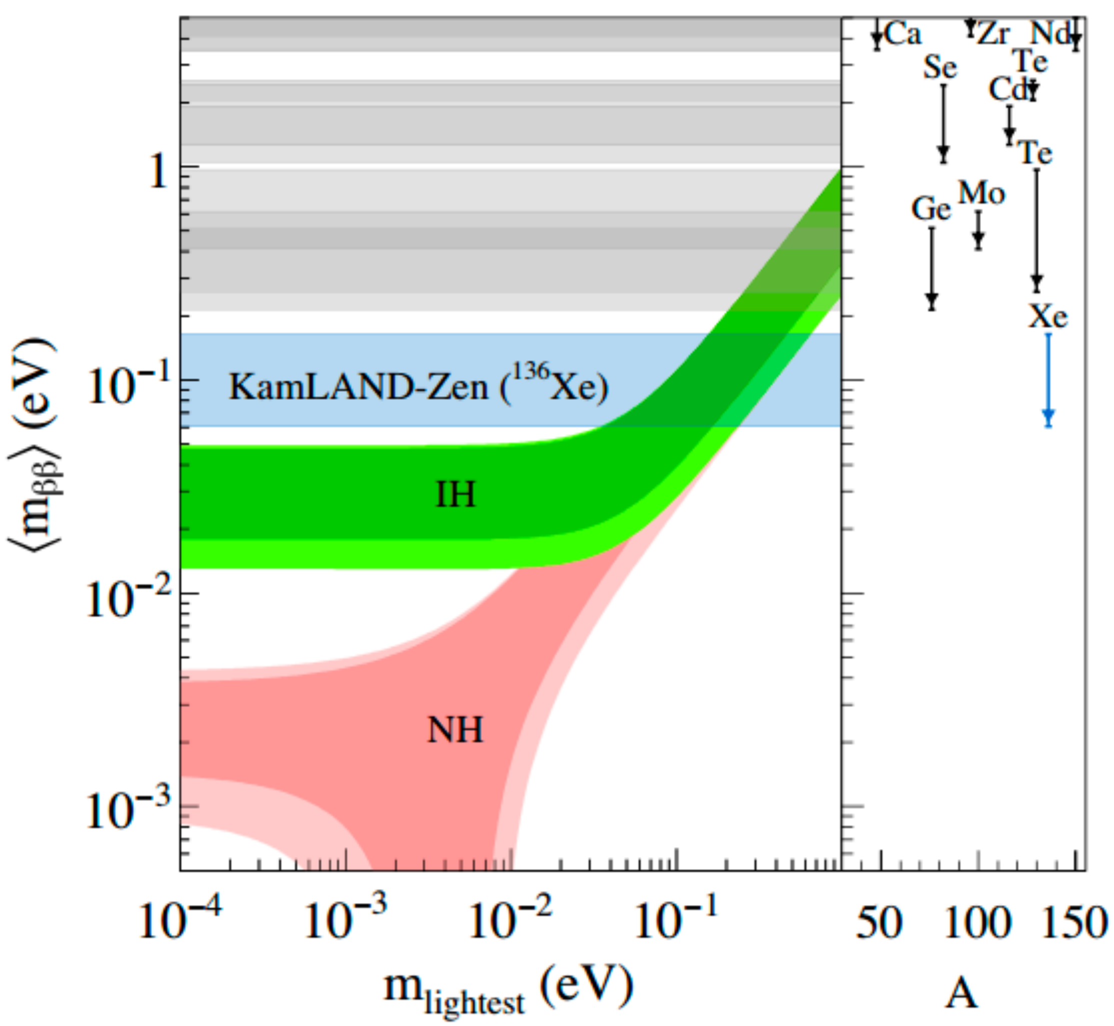
Lepton number violation

If lepton number is not conserved, then matter-antimatter asymmetry could be generated through leptogenesis

Fukugita, Yanagida, Phys. Lett. B 174 (1986)



Low-energy signature of lepton-number violation: $0\nu\beta\beta$



Gando et al (KamLAND-Zen) PRL 117 (2016)

Experiments directly measure half-lives $T^{0\nu}_{1/2}$ of specific nuclei ($A \geq 48$)

Using these results to constrain neutrino mass and mixing parameters requires nuclear matrix elements

$$(T^{0\nu}_{1/2})^{-1} = G^{0\nu}|\mathcal{M}^{0\nu}|^2 \langle m_{\beta\beta}\rangle^2$$

Phase space

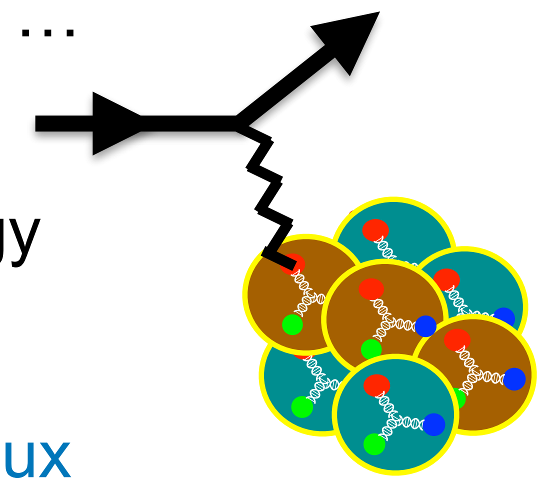
Nuclear matrix element

Neutrino masses and mixing

Challenging to calculate from first principles, but significant recent theory progress

Neutrino CP violation

Next-generation neutrino experiments DUNE and Hyper-Kamiokande aim to precisely measure neutrino CP violation, mass hierarchy, …



Relating measured final-state event rates to incoming neutrino energy distribution requires theory input on νA cross-section

Near-detector neutrino flux

$$\frac{N_{\rm near}(E_\nu)}{N_{\rm far}(E_\nu)} = \frac{\int dE'_\nu \Phi_{\rm near}(E'_\nu)\sigma(E'_\nu)}{\int dE'_\nu \Phi_{\rm far}(E'_\nu)\sigma(E'_\nu)}$$

Cross-section

Experimentally measured event rates

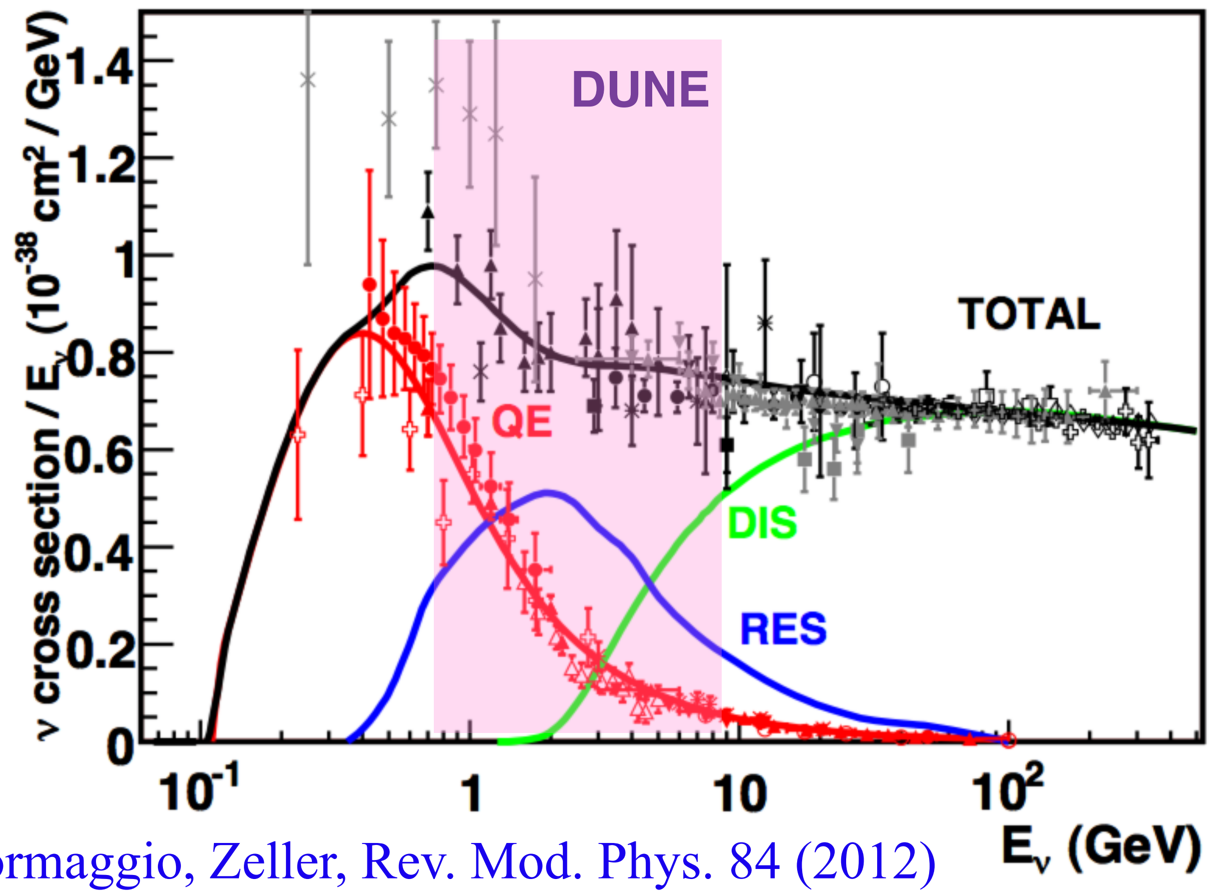
Far-detector flux (depends on oscillation parameters)

DUNE aims to have few-percent theory uncertainty

— estimates show going from 2% to 3% theory uncertainty means 50% longer runtime to measure CP violation at a given precision

Abi et al (DUNE), arXiv 1807.10334

Neutrino-nucleus scattering

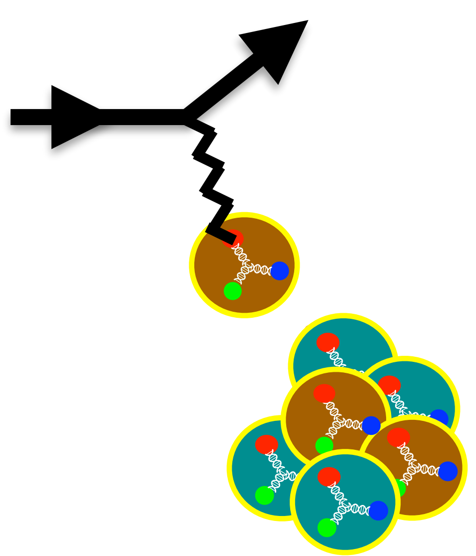


Formaggio, Zeller, Rev. Mod. Phys. 84 (2012)

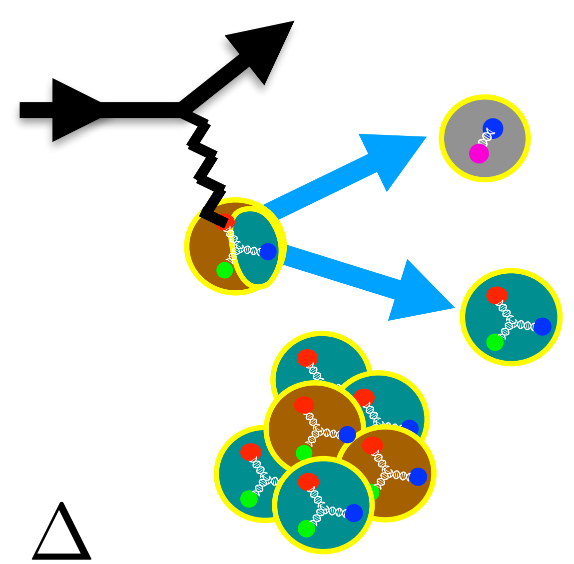
Accelerator neutrino flux covers a wide range of energies with different dominant physics processes:

- Quasi-elastic
- Resonance production
- Transition region
- Deep inelastic scattering

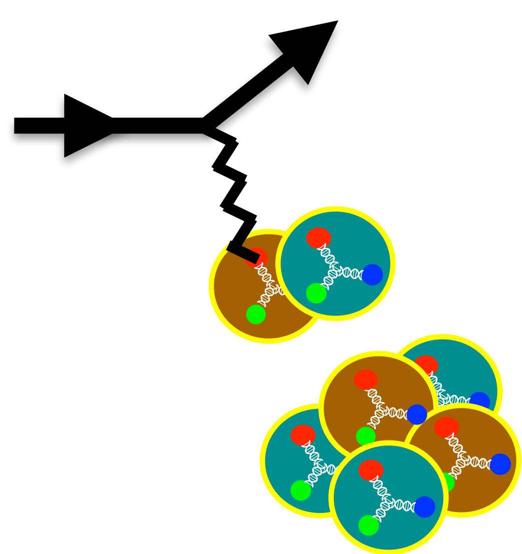
Nuclear models exist that can describe most of these regions, but precision x-sec predictions require precise knowledge of few-nucleon input parameters



Nucleon form factors



$N, \ \pi, \ \Delta$
transition form factors



Two-body currents

Lattice QCD, EFT, and νA

LQCD can provide results for few-nucleon quantities that inform nuclear effective theories and are complementary to experiment

LQCD → Nuclear EFT and many-body → Event generators

See USQCD νA white paper: Kronfeld et al Eur. Phys. J. A 55 (2019)

Easy for LQCD:

- Axial vs vector currents
- Isovector vs isoscalar
- Pions

Hard for LQCD:

- Large baryon number
- Real-time dynamics
- Multi-hadron states
- (Light quark masses)

Lattice QCD and νA

νA scattering amplitudes factorize into leptonic and hadronic parts

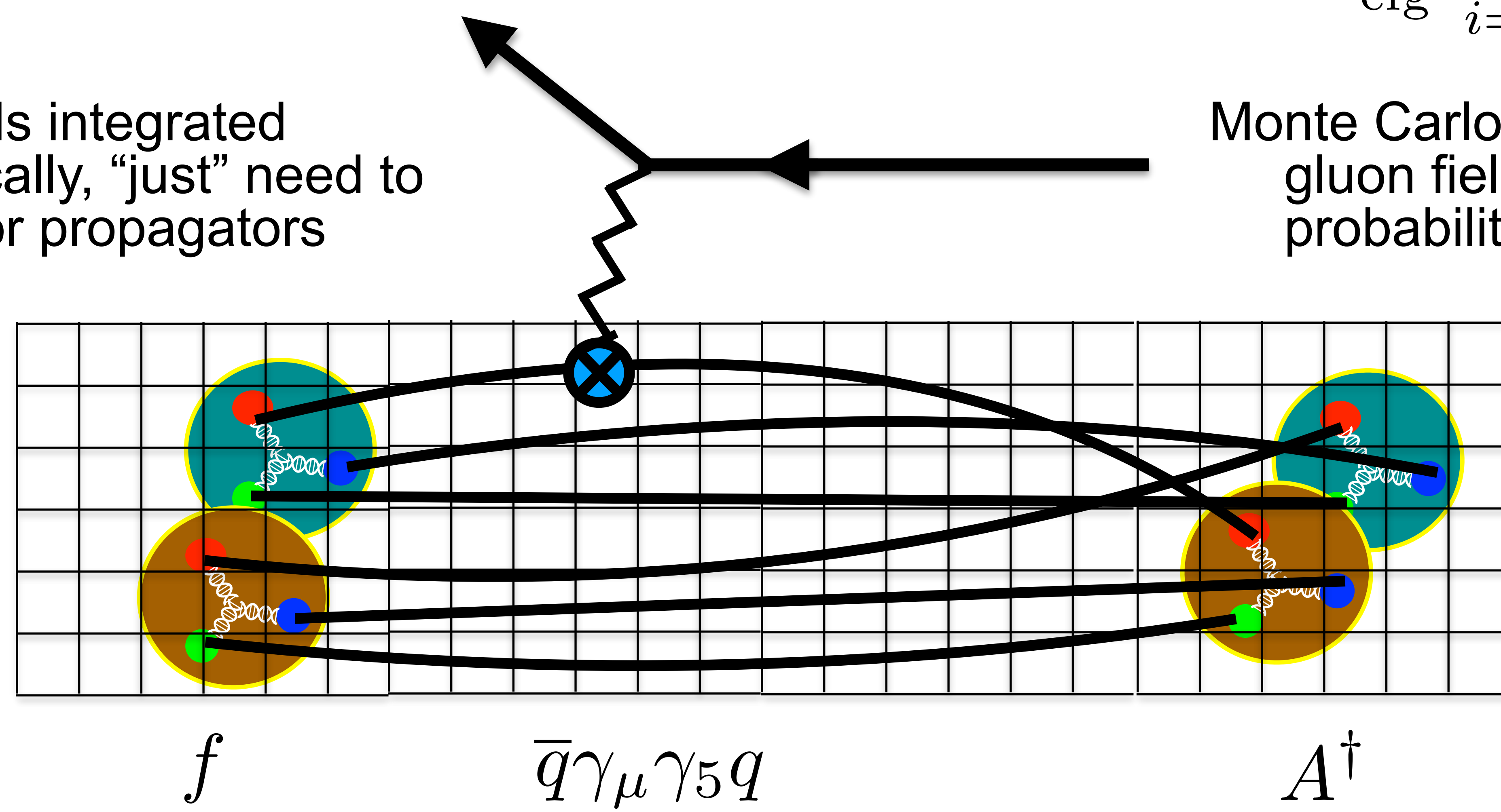
$$\mathcal{M}_{\nu A \to \ell f} \propto \left(\overline{u}_\ell \gamma_\mu \gamma_5 u_\nu \right) \langle f | \, \overline{q} \gamma_\mu \gamma_5 q \, | A \rangle + \dots$$

Generic Euclidean hadronic matrix elements calculable (in principle) using lattice QCD

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\overline{q} \mathcal{D}q \; e^{-S_{QCD}(U,q,\overline{q})} \; \mathcal{O}(U,q,\overline{q}) \approx \frac{1}{N_{\text{cfg}}} \sum_{i=1}^{N_{\text{cfg}}} \mathcal{O}(U_i)$$

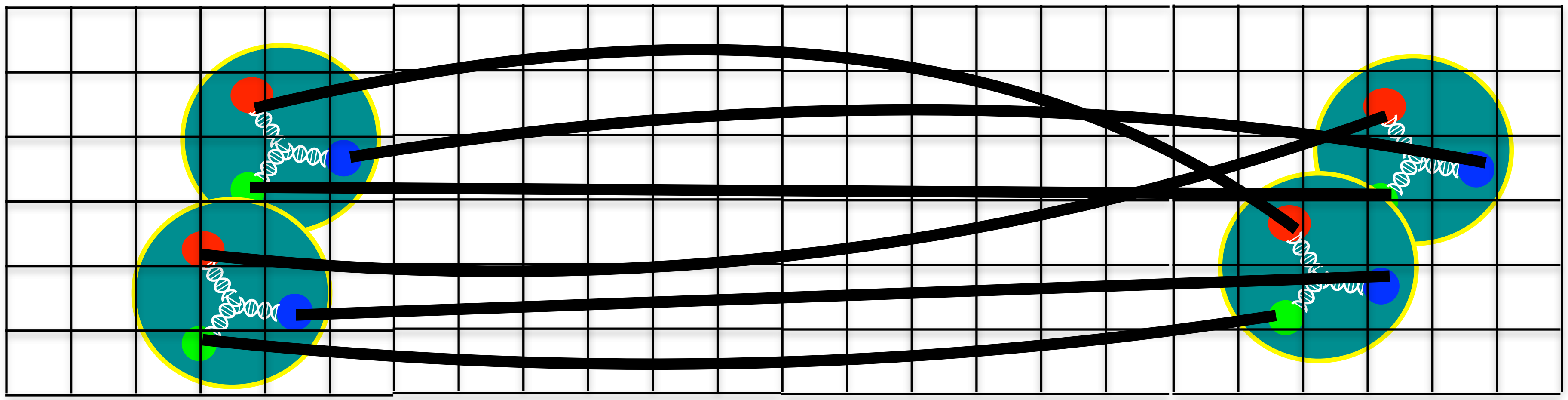
Quark fields integrated analytically, “just” need to solve for propagators

Monte Carlo sample gluon fields with probability $\propto e^{-S_{eff}}$



LQCD and nuclear matrix elements

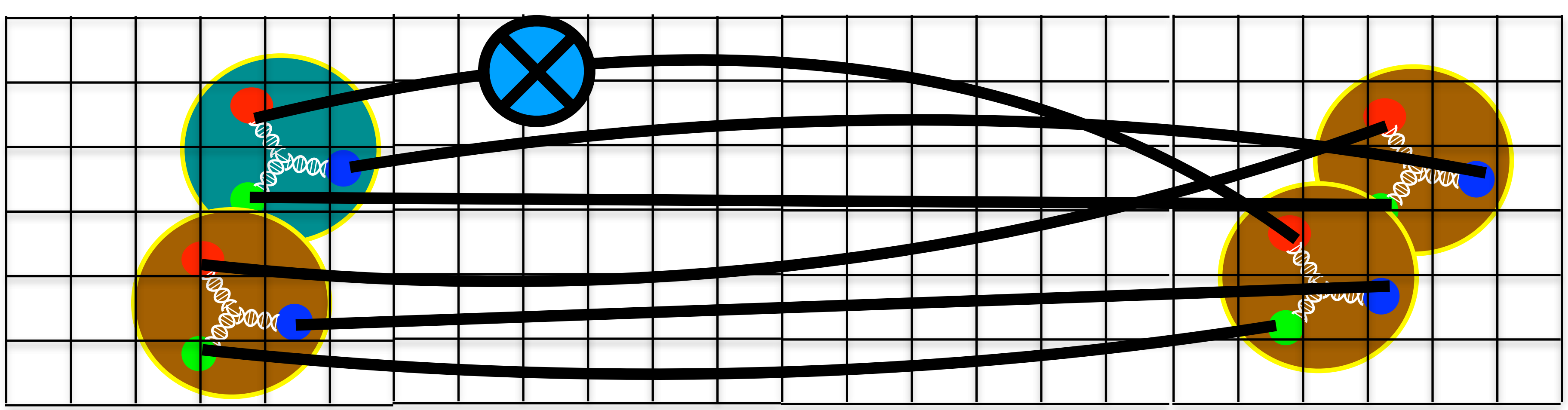
LQCD spectrum determined from 2-point correlation functions



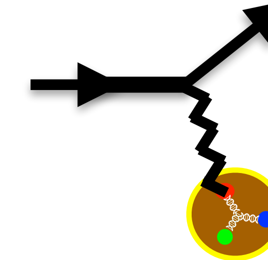
$$C_A(t) = \langle A(t) A^\dagger(0) \rangle = \sum_n \langle 0|A(0)e^{-Ht}|n\rangle \langle n|A^\dagger(0)|0\rangle + \ldots$$

$$= \sum_n |Z_n|^2 e^{-E_n t}$$

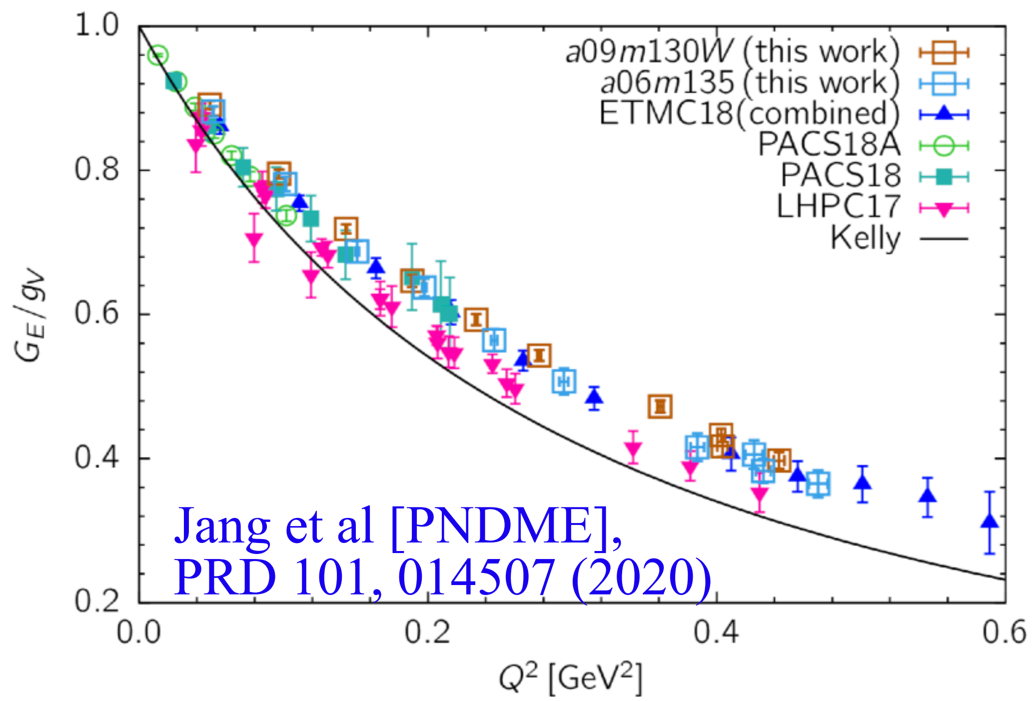
Nuclear matrix elements determined from 3-point correlation functions including a local operator insertion

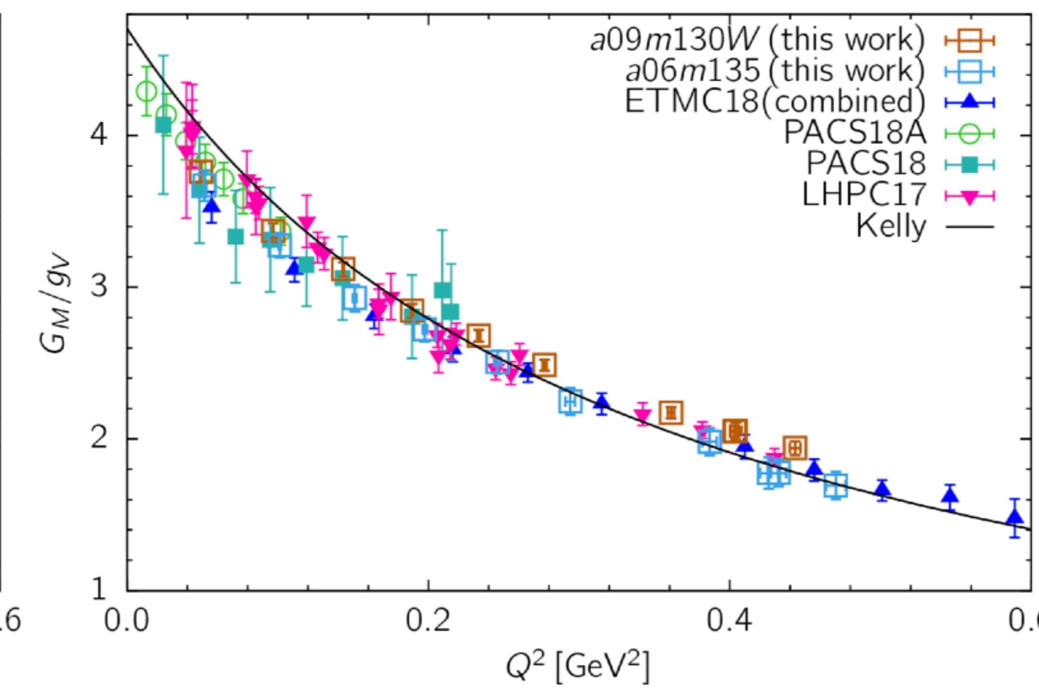


Nucleon form factors



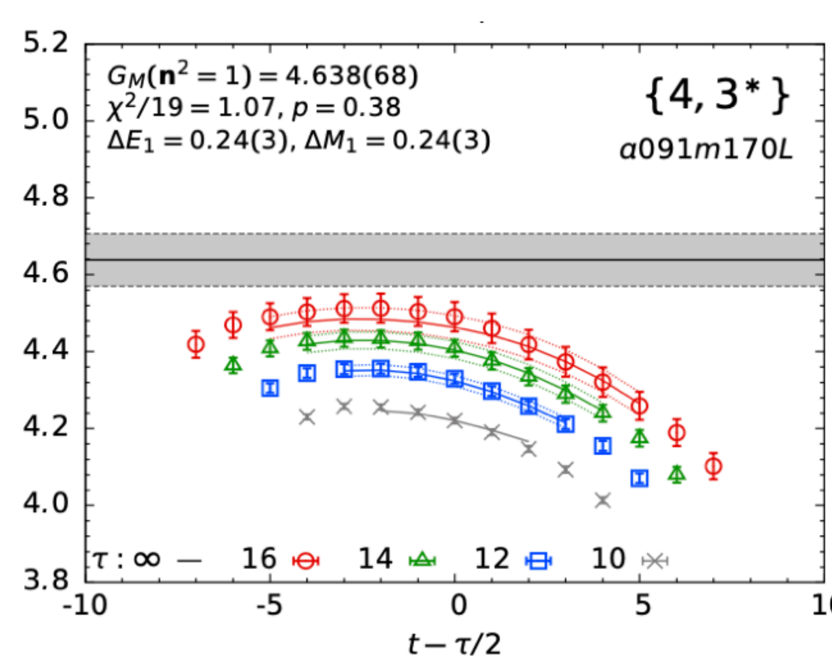
Vector and axial form factors recently calculated using nearly physical quark masses:

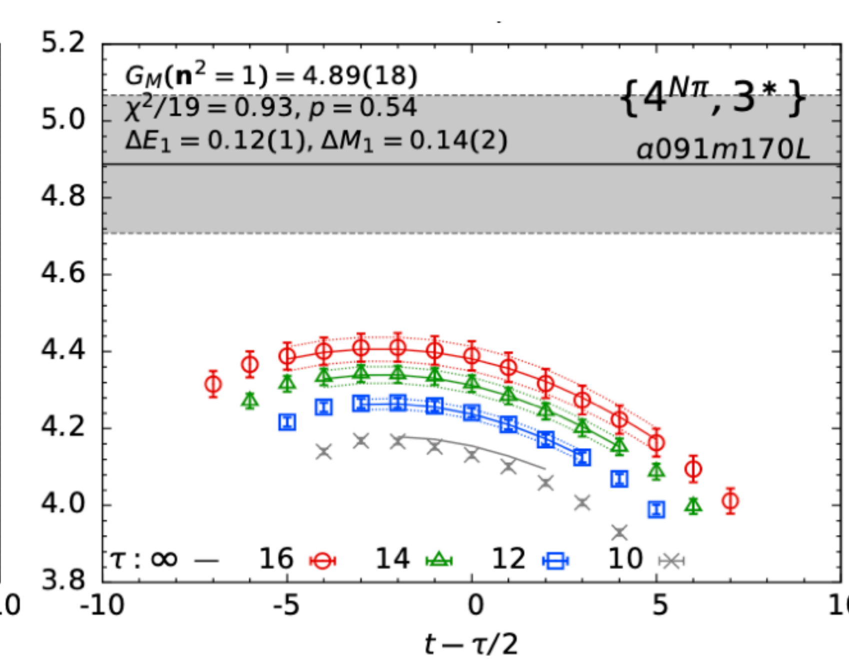




Remaining LQCD systematic uncertainties arise from lattice spacing effects, finite-volume effects, **excited-state effects**

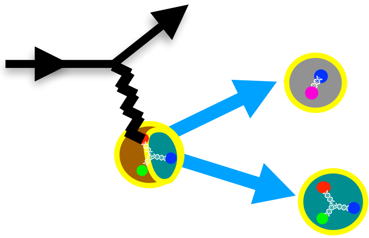
Recent vector / axial form factor studies show the importance of $N\pi$ excited-state effects in nucleon form factor calculations with light quark masses



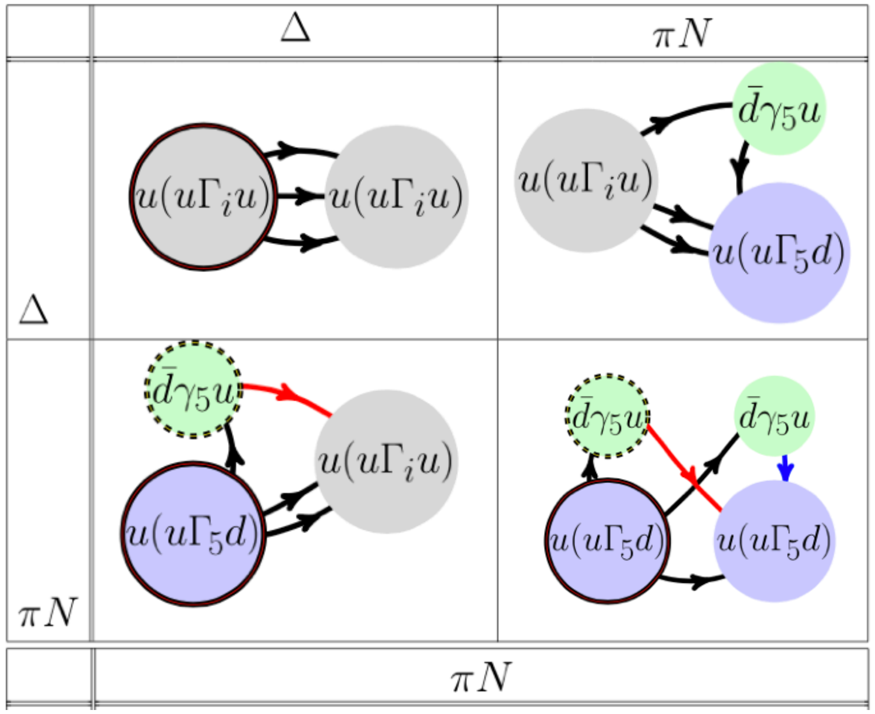


Park et al [NME], arXiv:2103.05599

$N\pi$ scattering

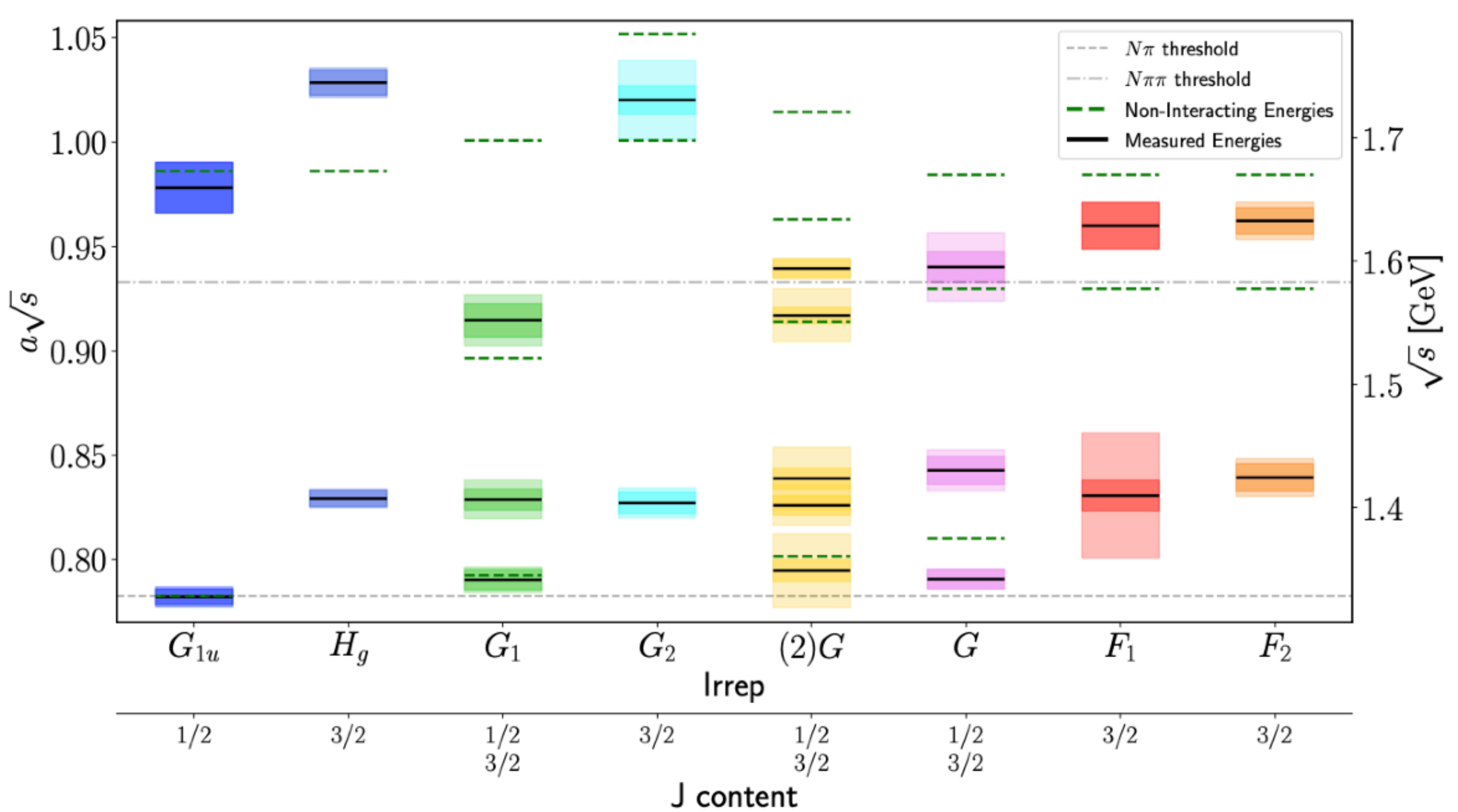


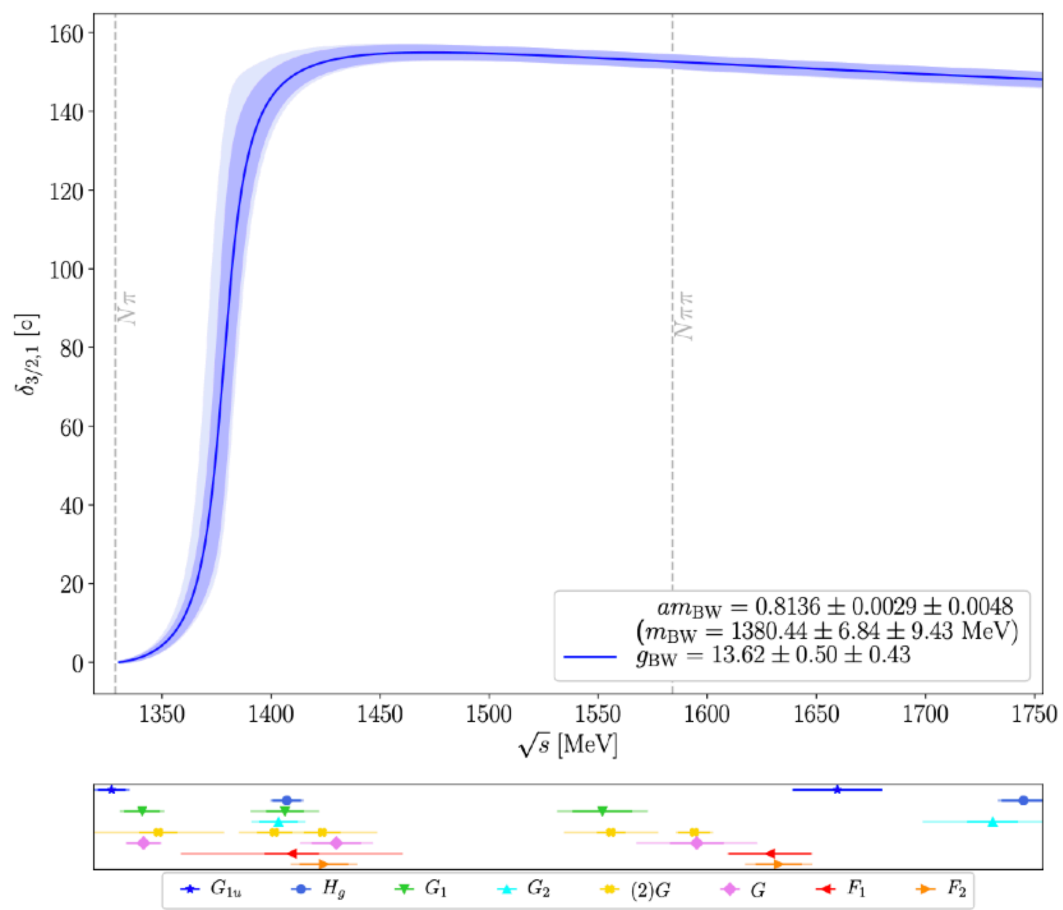
Recent calculations in *I* = 3/2 channel including Δ and $N\pi$ interpolating operators use variational methods to extract ground- and excited-states in many angular momentum channels (cubic irreps)



Silvi et al, PRD 23 (2021)

Finite-volume quantization conditions relate energy levels to p-wave $N\pi$ scattering phase shifts

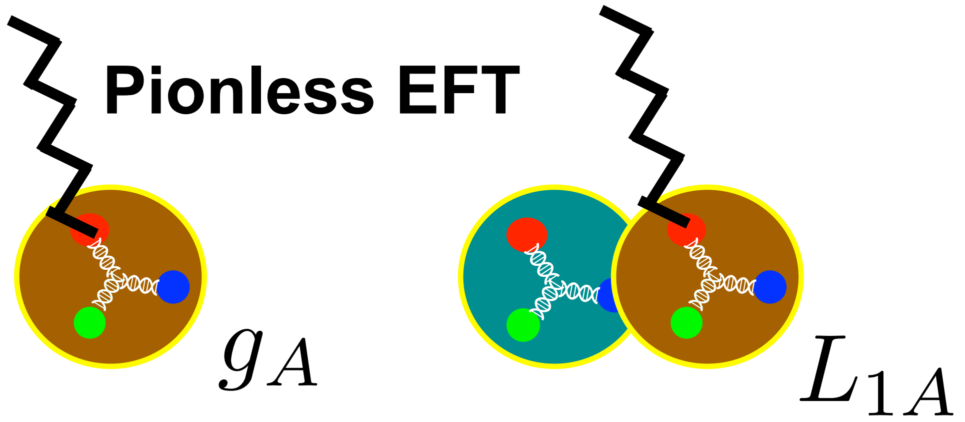




Axial currents in nuclei

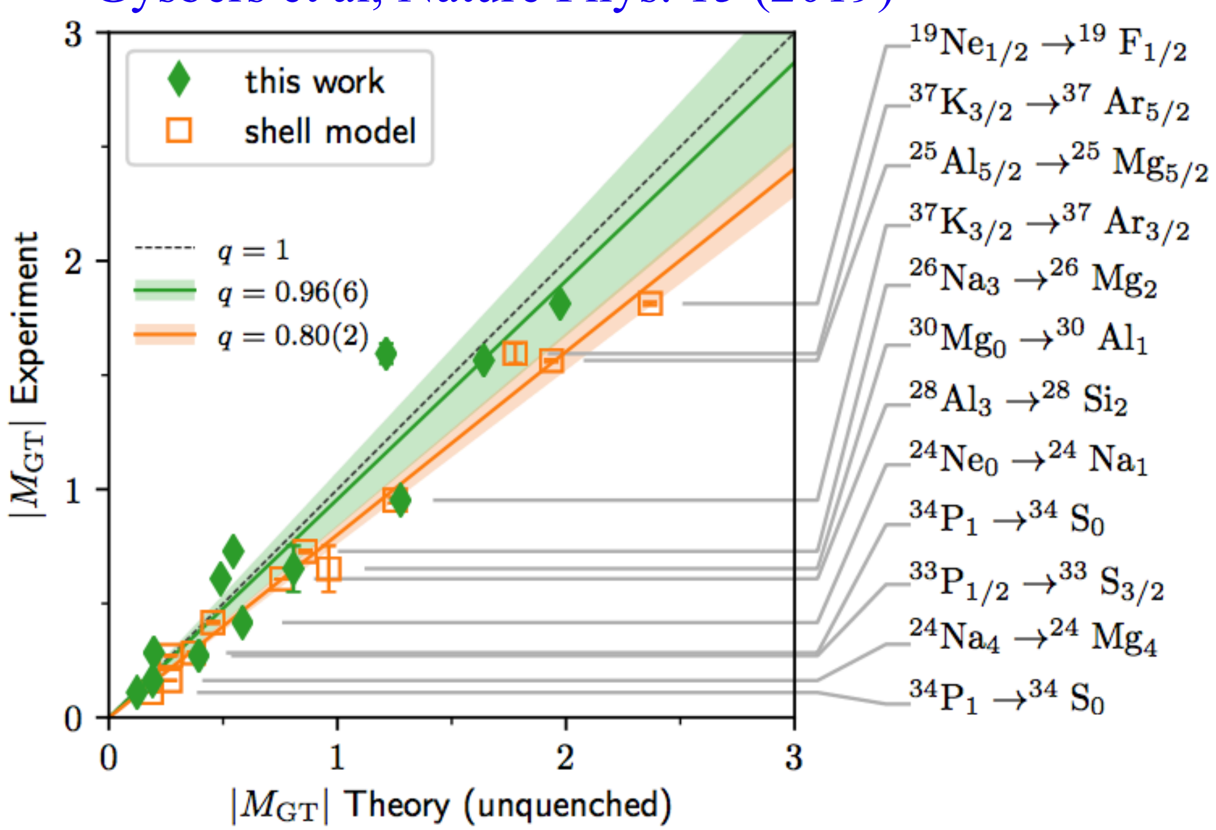
Axial-current responses of nucleons are modified in nuclei

Modern calculations including multi-nucleon correlations and currents with e.g. chiral EFT can reproduce experiment without "quenching" g_A

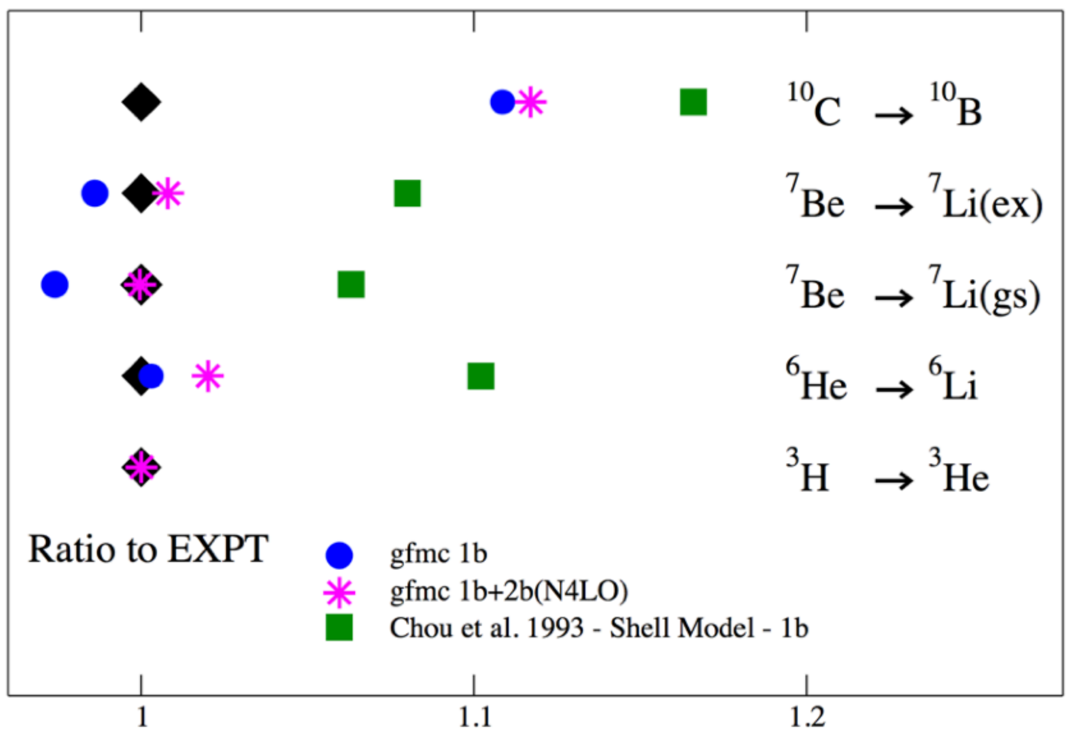


Few-nucleon LQCD results can constrain two-body currents in nuclear models and EFTs

Gysbers et al, Nature Phys. 15 (2019)



Pastore et al, PRC 97 (2018)

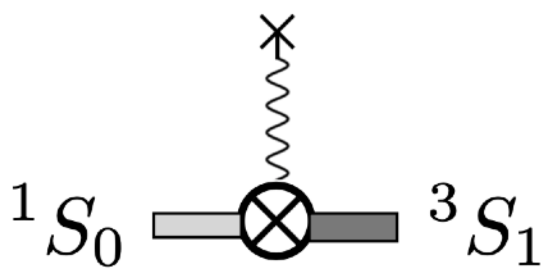


Proton-proton fusion

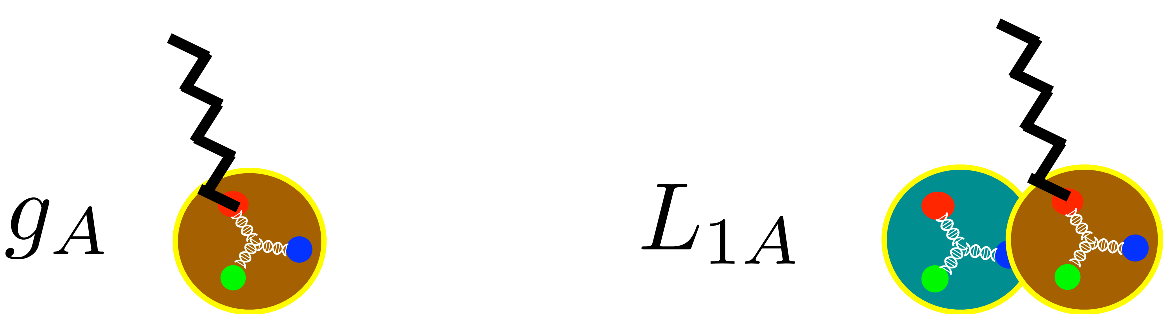
Axial current transition matrix element between spin-singlet and spin-triplet np systems computed using fixed-order background fields

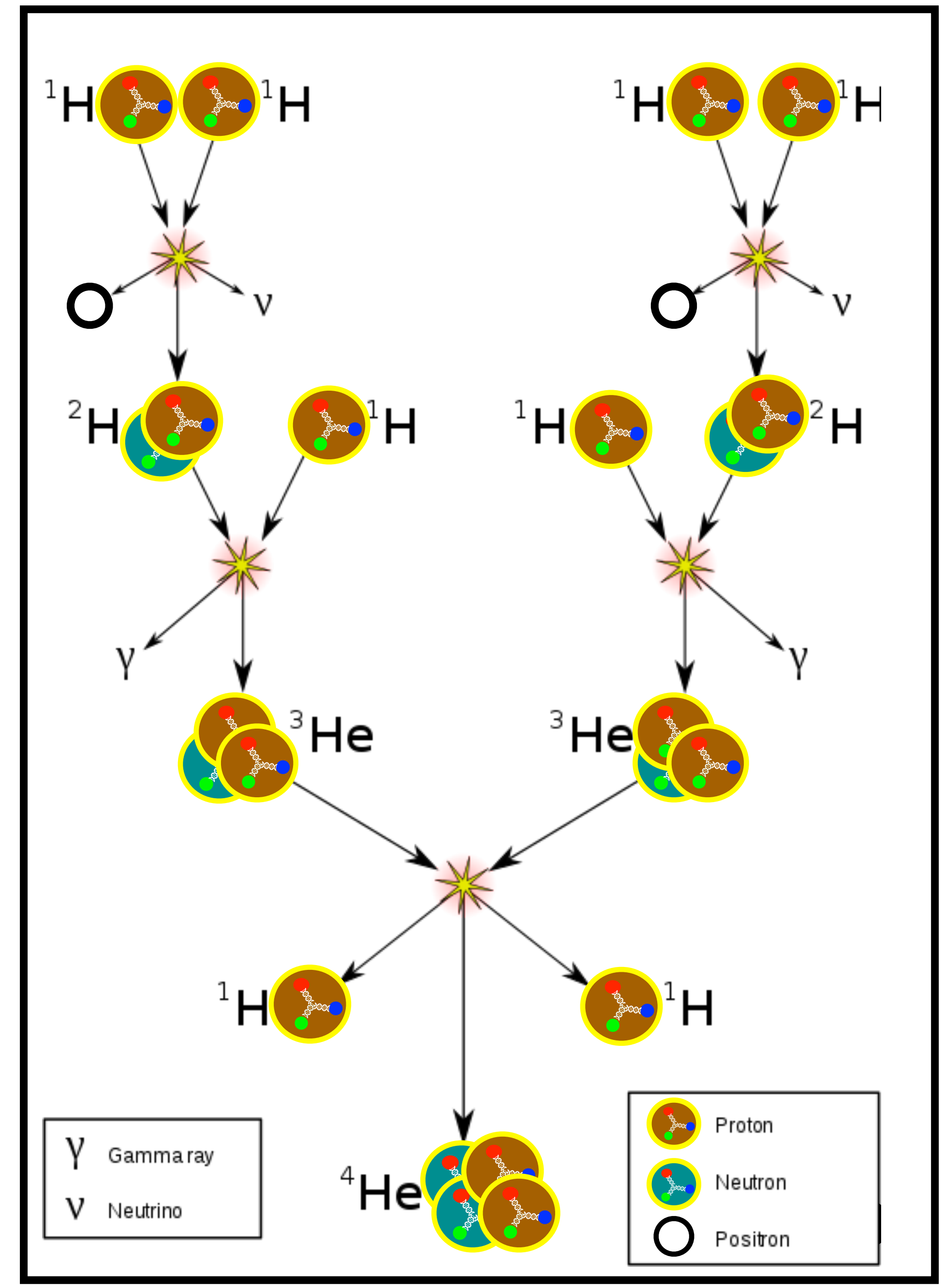
Savage, MW et al [NPLQCD], PRL 119 (2017)

LQCD results matched to pionless EFT by computing same background-field correlation function



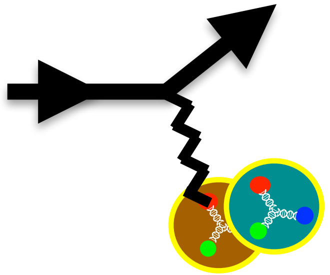
Results used to constrain LEC for two-body axial current operator in pionless EFT





Same operator relevant for proton-proton fusion and other reactions, future LQCD calculations could improve phenomenological predictions

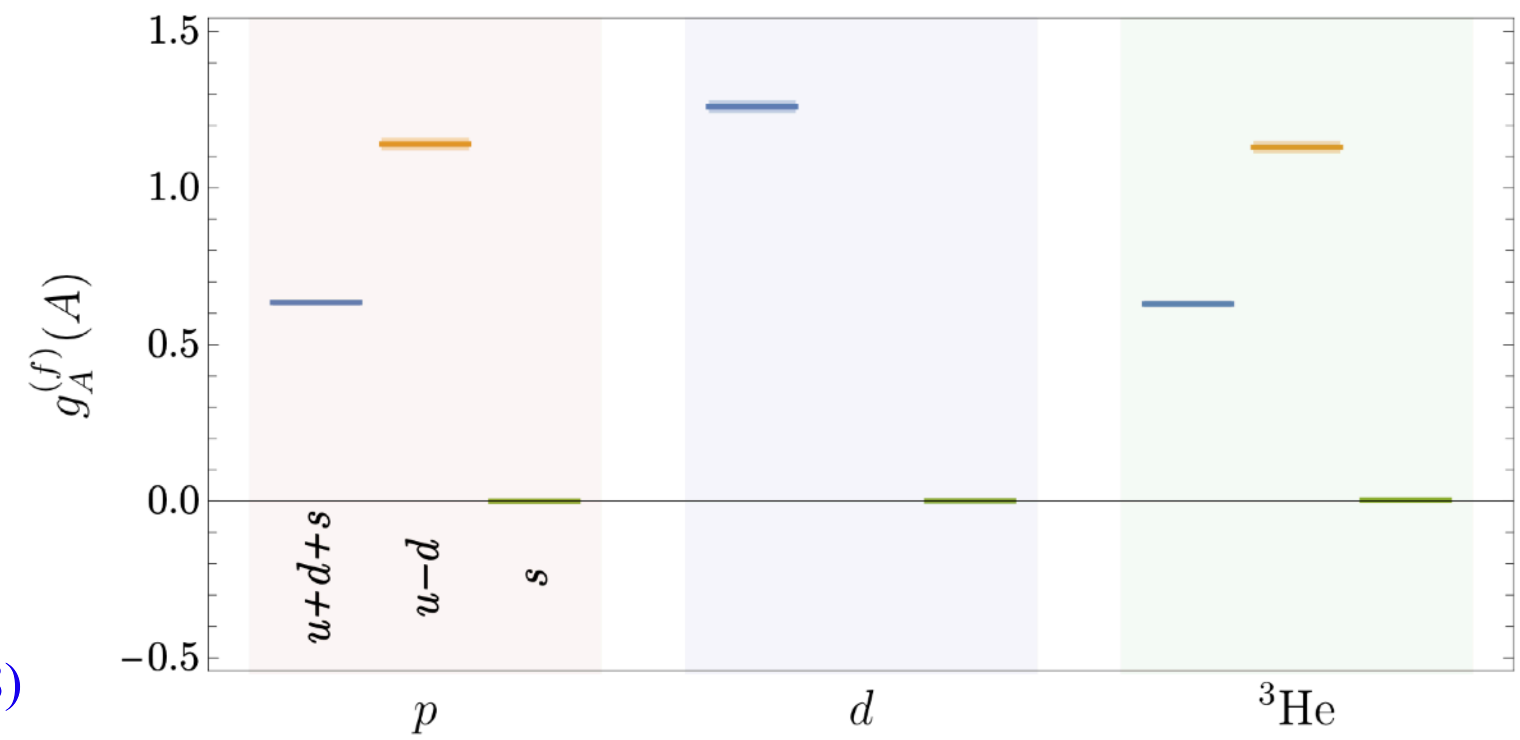
Axial matrix elements

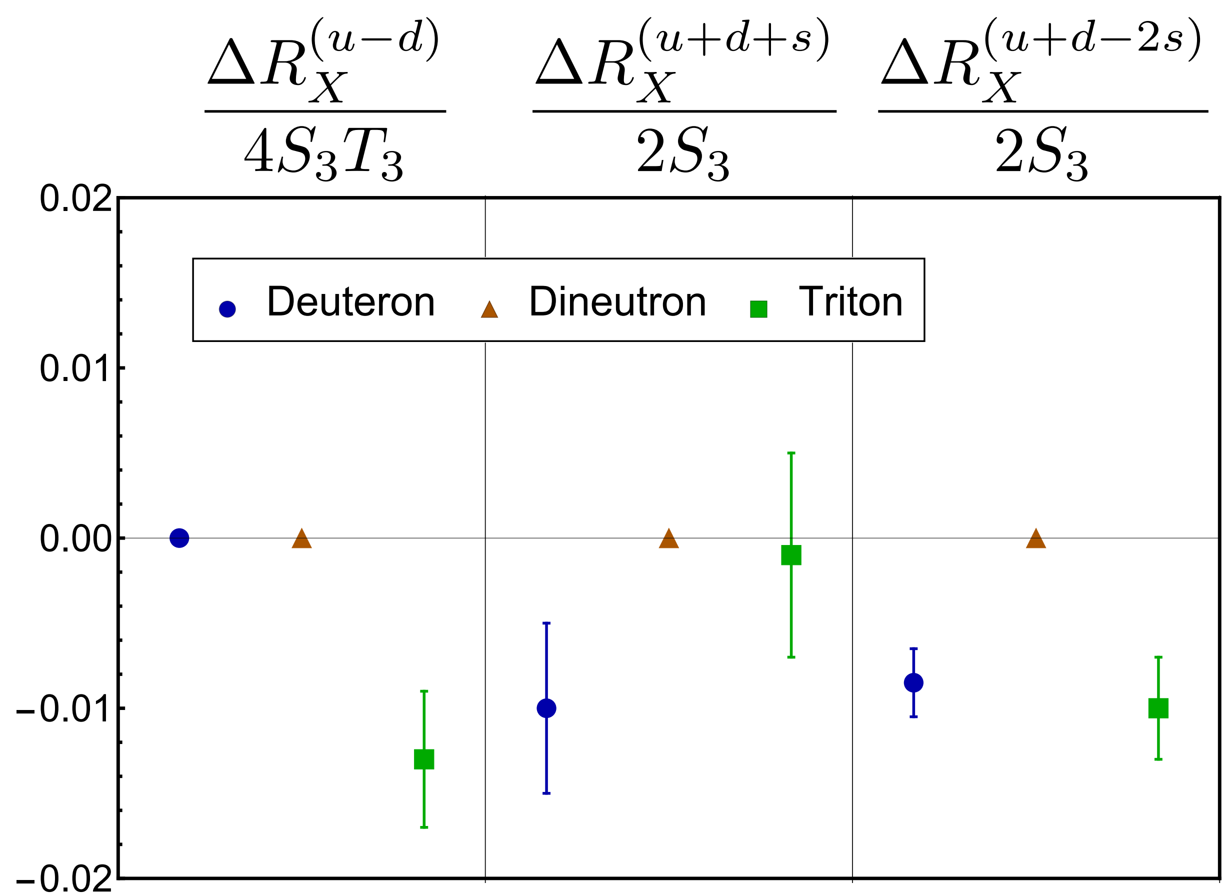


Flavor decomposition of axial matrix elements of up to three nucleon systems computed with

$m_\pi = 806$ MeV

Chang, MW et al [NPLQCD], PRL 120 (2018)

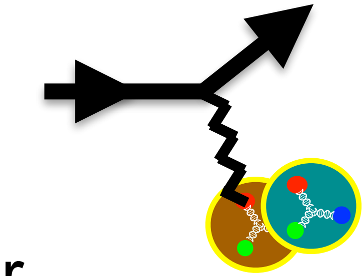


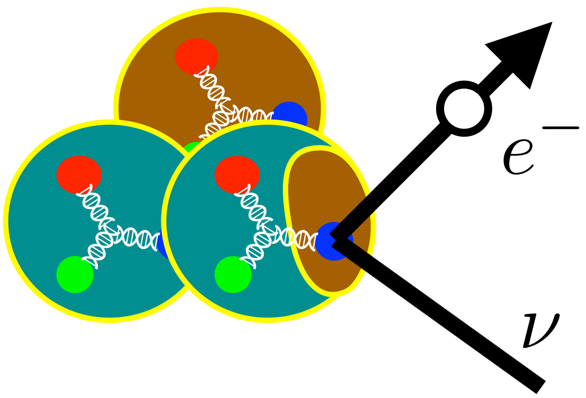


$N_f = 3,\ m_\pi = 806(9)\ \text{MeV},\ a = 0.145(2)\ \text{fm}$

Fractional differences from naive shell model expectations show that multi-nucleon correlations lead to percent-level effects on axial charges of light nuclei for these quark masses

Triton β decay





Triton β - decay rate governed by Gamow-Teller matrix element

$$g_A(^3\mathrm{H}) = |\langle ^3\mathrm{He}|A_3^+|^3\mathrm{H}\rangle| = |\langle ^3\mathrm{H}|A_3^+|^3\mathrm{H}\rangle|$$

Computed in ChEFT   Baroni et al, PRC 98 (2018)

After fitting LECs to experimental triton β-decay rate predicts

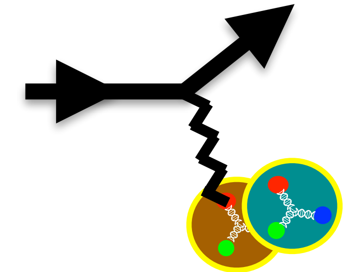
$$\frac{|\langle ^3\mathrm{He}|A_3^+|^3\mathrm{H}\rangle|}{g_A} = 0.951(13)$$

Deviations from 1 arise from two-body currents and multi-nucleon interactions

NLO calculations in pionless EFT relate nuclear effects to the two-body axial current coupling L_{1A} appearing in proton-proton fusion

De-Leon, Platter, Gazit (2016)

Triton β decay from LQCD

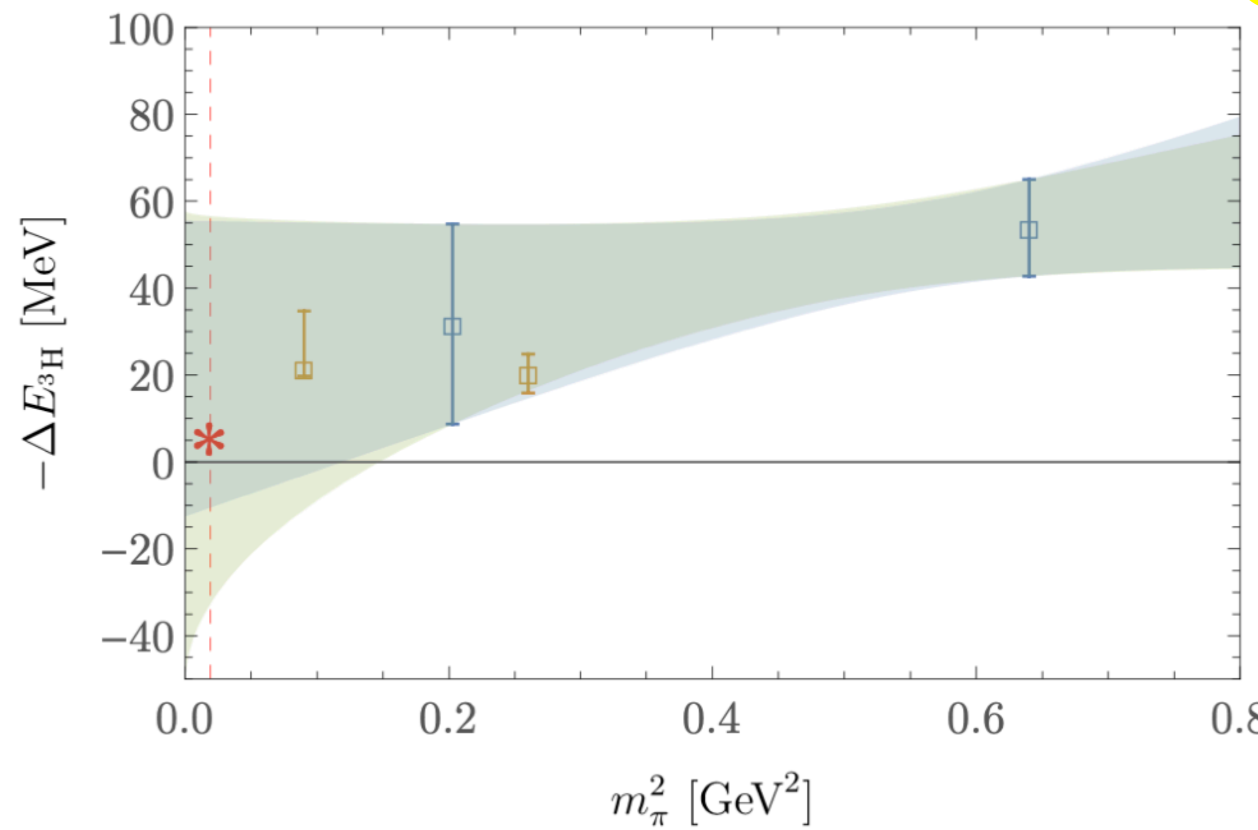


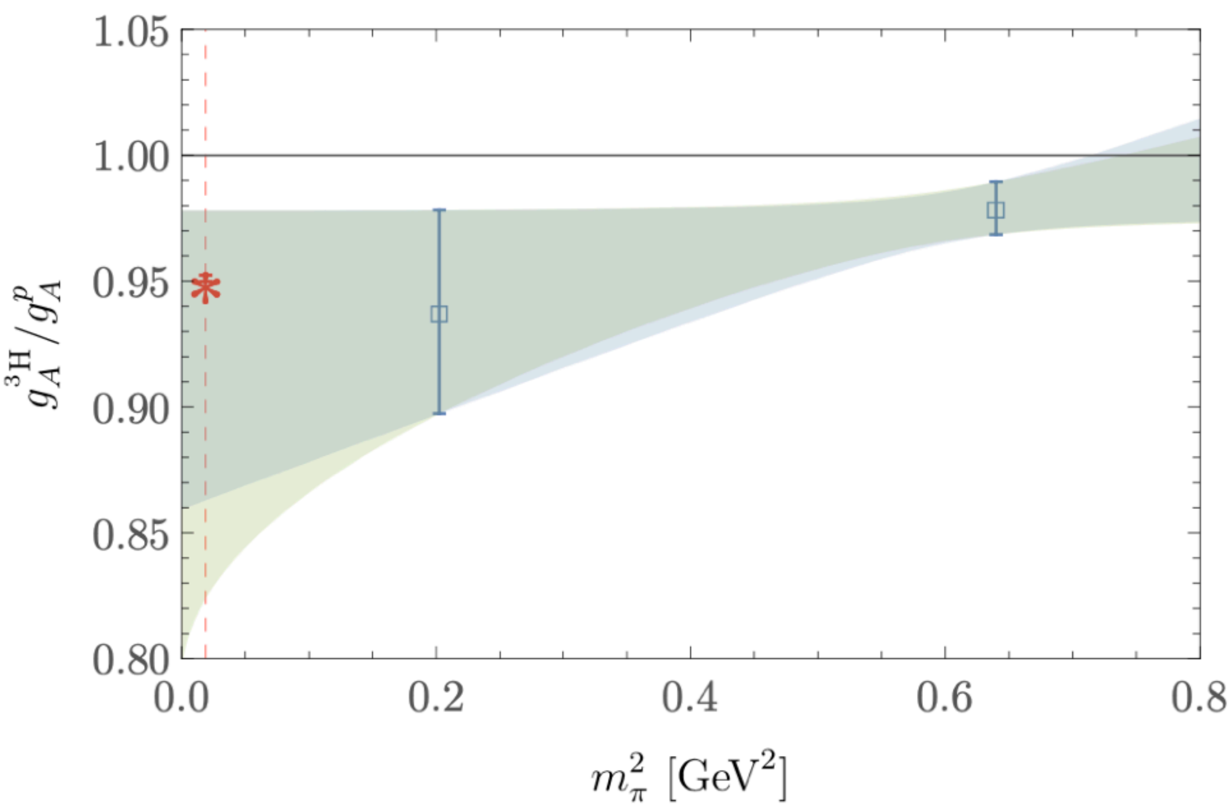
LQCD calculations of triton recently performed using $m_\pi = 450$ MeV

Parreño, MW et al [NPLQCD] PRD 103 (2021)

Signal-to-noise problem makes calculations exponentially noisier at lighter quark masses

Results consistent with bound triton obtained on 3 volumes





Parreño, MW et al [NPLQCD] PRD 103 (2021)

Axial current matrix element calculations with $m_\pi = 450$ MeV permit preliminary extrapolation to physical point

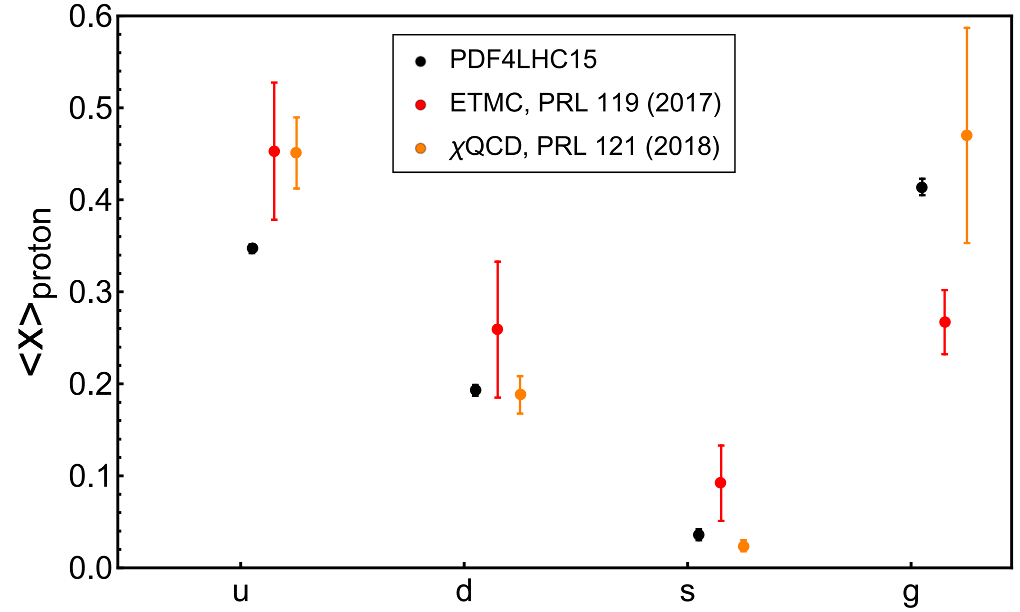
Several systematic uncertainties remain, but encouraging agreement with experiment seen

Matching to finite-volume pionless EFT used to constrain L_{1A}

Detmold and Shanahan, PRD 103 (2021)

PDFs and LQCD

LQCD can also compute quantities relevant to high-energy scattering



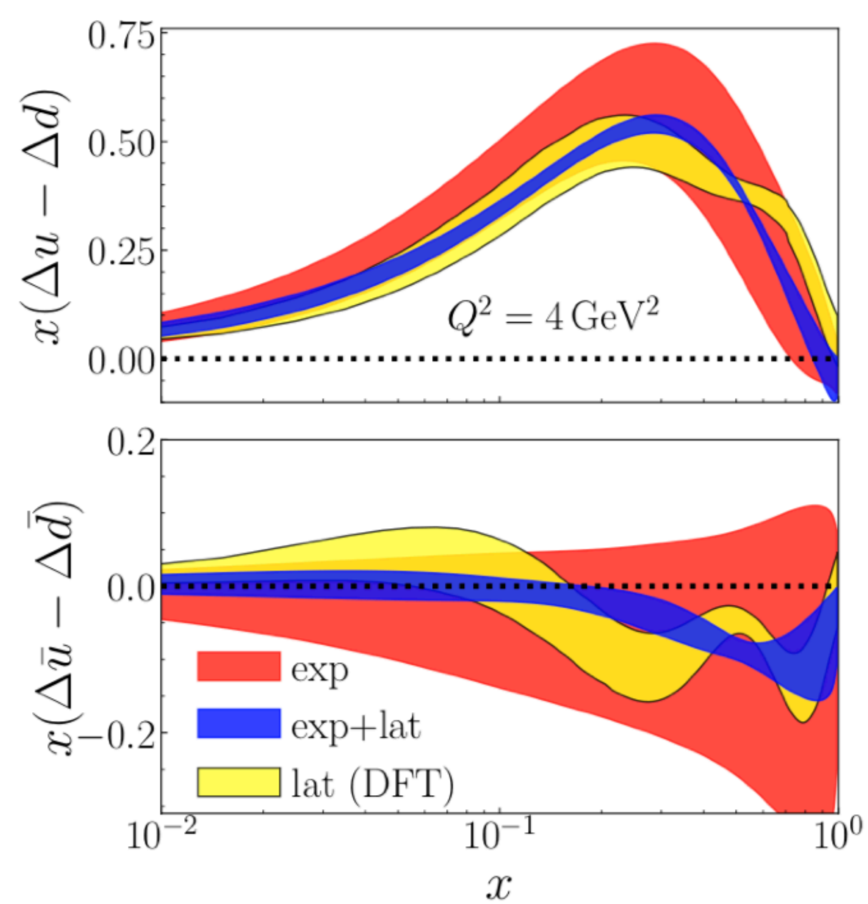
$\langle x \rangle^q_{\text{proton}}$ and $\langle x \rangle^g_{\text{proton}}$ calculated by several groups

Review: Lin et al, Prog. Part. Nucl. Phys. 100 (2018)

Large momentum effective theory connects Euclidean matrix elements to light-cone PDFs

Review: Ji et al, Rev. Mod. Phys. 93 (2021)

Current LQCD results can improve global analyses of isovector polarized PDFs



Bringewatt et al [JAM], arXiv:2010.00548

Nuclear momentum fractions

First calculations of gluon and isovector quark momentum fractions of light nuclei

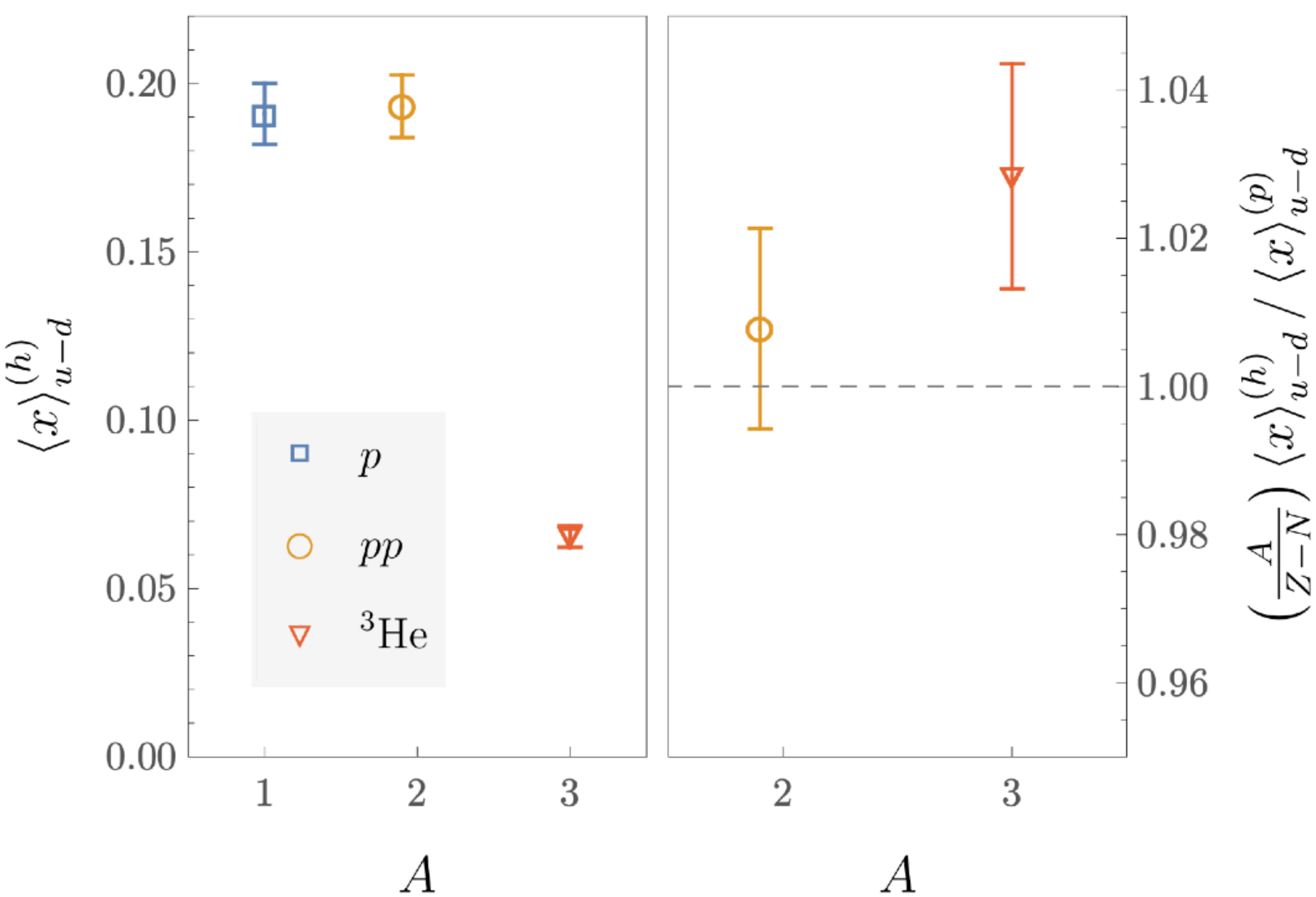
Winter, MW et al [NPLQCD], PRD 96 (2017)

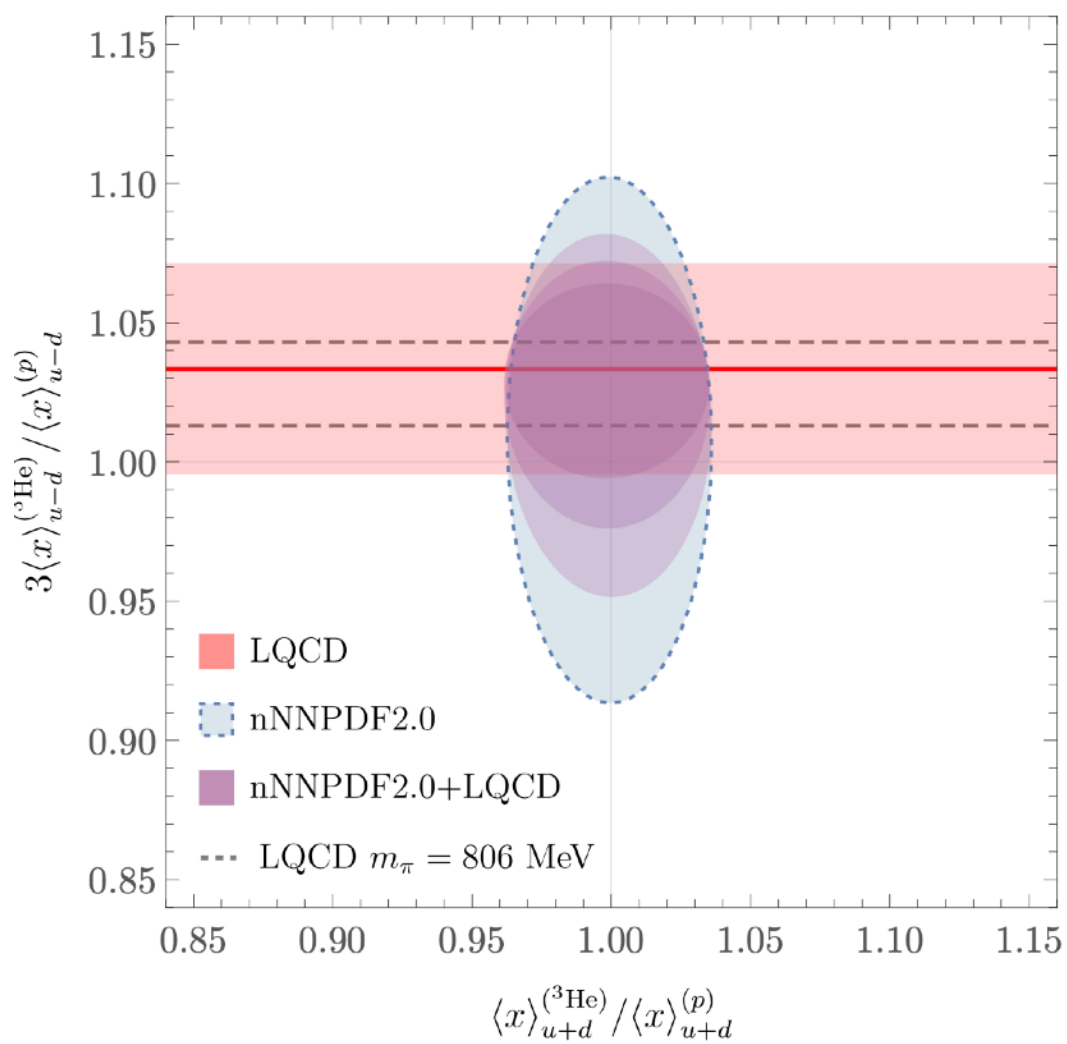
Detmold, MW et al [NPLQCD] PRL 126 (2021)

Results matched to poinless EFT to determine two-body current operator that governs isovector EMC effects relevant to neutrino DIS

Cloët, Bentz, Thomas, PRL 102 (2009)

Although systematic uncertainties are not fully controlled (one lattice spacing, volume, quark mass, …) demonstrates potential for LQCD to usefully constrain nuclear PDFs





Beyond-Standard-Model Interactions

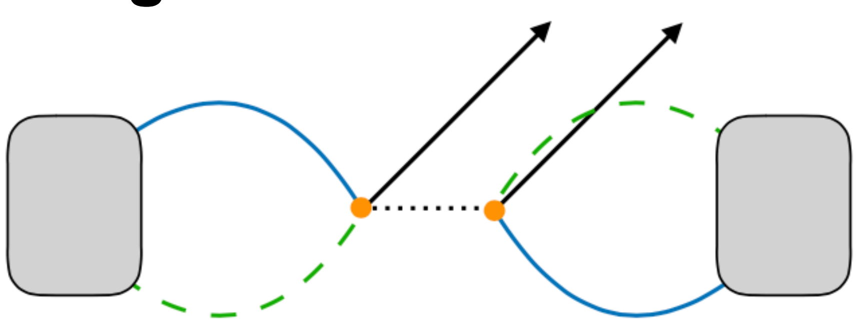
Nuclear matrix elements for $2\nu\beta\beta$ calculated similarly with background fields

$\langle pp | A_3^+ A_3^+ | nn \rangle$ Shanahan, MW et al [NPLQCD], PRL 119 (2017)

Pion analogs of $0\nu\beta\beta$ such as $\pi^- \to \pi^+ e^- e^-$ computed

Short distance Nicholson et al, PRL 121 (2018)

Long distance Feng et al, PRL 122 (2019) Tuo, Feng, and Jin, PRD 100 (2019) Detmold and Murphy, arXiv:2004.07404

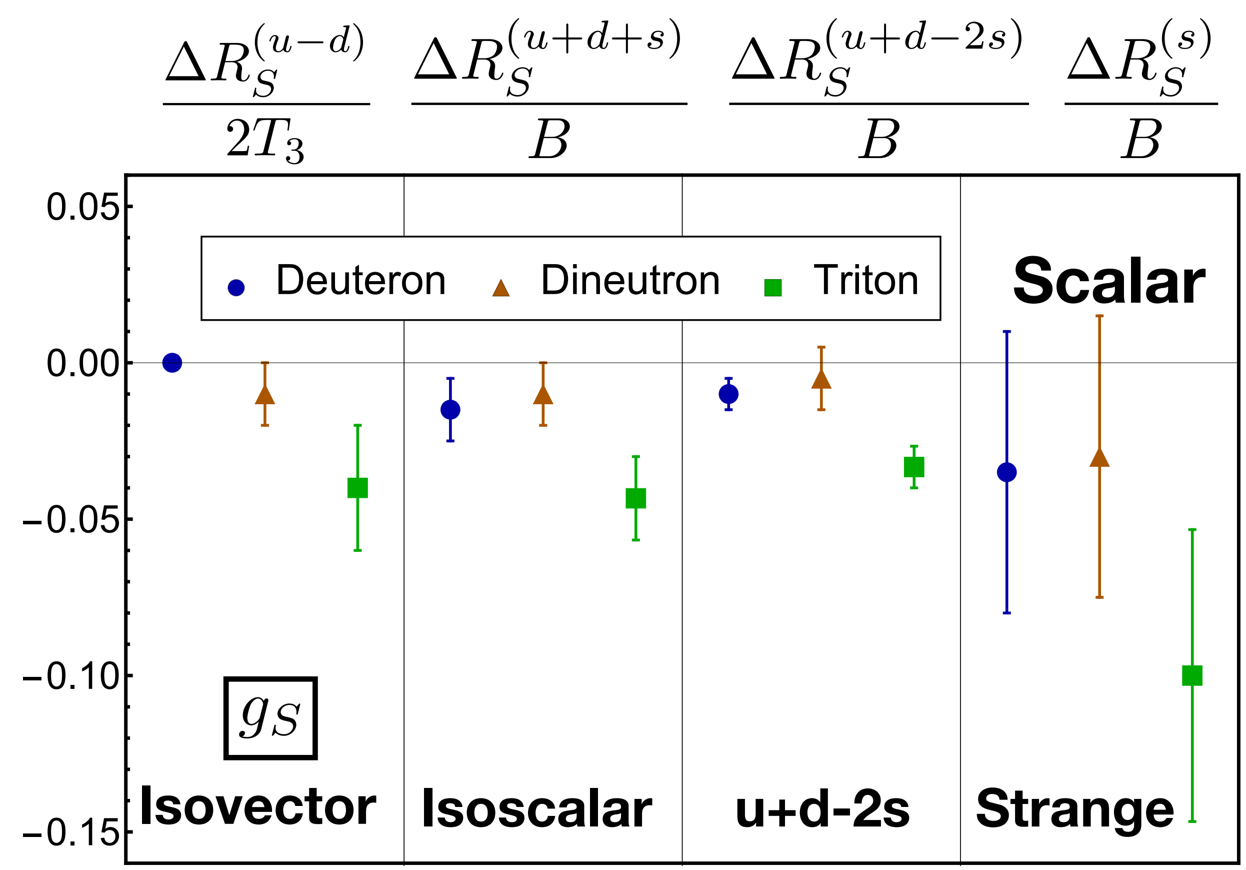


Other nuclear matrix elements of BSM currents computed with $m_\pi \approx 806$ MeV

Chang, MW et al [NPLQCD], PRL 120 (2018)

Scalar current nuclear matrix elements relevant to dark matter direct detection

Tensor current nuclear matrix elements relevant to nuclear electric dipole moments



Systematic uncertainties

Several systematic uncertainties remain to be quantified in detail

- Heavier than physical quark masses only
- One lattice spacing
- Excited-state effects

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Gap between ground and two-nucleon finite-volume "scattering" states becomes small for large volumes, ground-state dominance relies on overlap factors

$$Z_0 e^{-E_0 t} \left(1 + \frac{Z_1}{Z_0} e^{-\delta t} + \dots \right) \qquad \delta \sim \frac{4\pi^2}{ML^2}$$

For non-positive-definite correlation functions, cancellations between the ground and excited-state could in principle conspire to form a "false plateau"

See e.g. Iritani et al, JHEP 10 (2016)

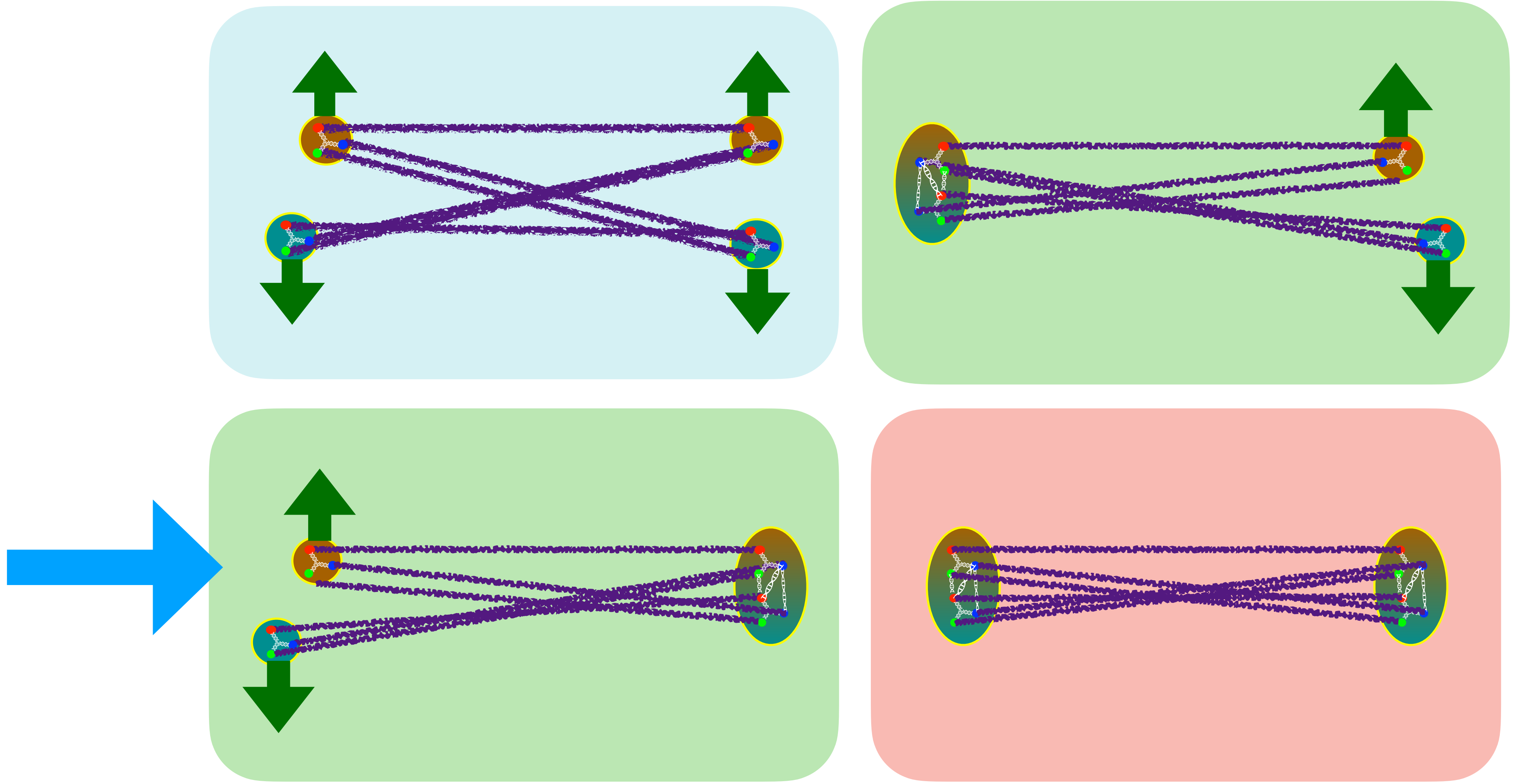
First studies using positive-definite correlation functions (enabled by distillation / stochastic LapH) give results that suggest tensions with previous studies

Francis et al, PRD 99 (2019) Hörz et al, PRC 103 (2021) Green et al, PRL 127 (2021)

The variational method

Correlation-function matrices for an interpolator set including both local "hexaquark" and bilocal "dibaryon" operators can generalize calculations performed to date

Variational bounds on energy spectrum obtained by diagonalizing these matrices



All LQCD nuclear matrix element calculations

Although application of variational methods to multi-nucleon systems has long been advocated, it has only recently become computationally feasible through methods such as distillation and propagator sparsening

Peardon et al PRD 80 (2009)

Morningstar et al PRD 83 (2011)

Detmold, MW, PRD 104 (2021)

Li et al, PRD 103 (2021)

Hexaquark operators

Known from $\pi\pi$ scattering studies near the ρ resonance that local and nonlocal operators can be nearly orthogonal

Dudek et al, PRD 87 (2013)

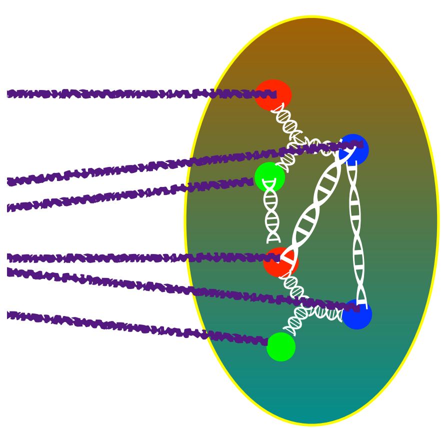
Wilson et al, PRD 92 (2015)

$$\overline{q}(x)\Gamma q(x) \qquad \pi(\vec{p}_1)\pi(\vec{p}_2)$$

Calculations with $t \sim$ few fm neglecting one type of operator show plateau-like behavior but energy spectra with "missing levels" (compared to more complete calculations)

Analog of $\overline{q}(x)\Gamma q(x)$ operators - local (up to Gaussian smearing) "hexaquark"

$$H_{0\mathfrak{n}s}(t) = \sum_{\vec{x}\in\Lambda_S} \psi_{\mathfrak{n}}^{[H]}(\vec{x})\varepsilon^{abcdef}\frac{1}{2}\Big[p_{1s}^{abc}(\vec{x},t)n_{2s}^{def}(\vec{x},t) - p_{2s}^{abc}(\vec{x},t)n_{1s}^{def}(\vec{x},t)$$
$$+n_{1s}^{abc}(\vec{x},t)p_{2s}^{def}(\vec{x},t) - n_{2s}^{abc}(\vec{x},t)p_{1s}^{def}(\vec{x},t)\Big]$$



Quark exchange symmetries very useful for reducing the number of weights

Detmold and Orginos, PRD 87 (2013) $\qquad 2880 \to 21$

Dibaryon operators

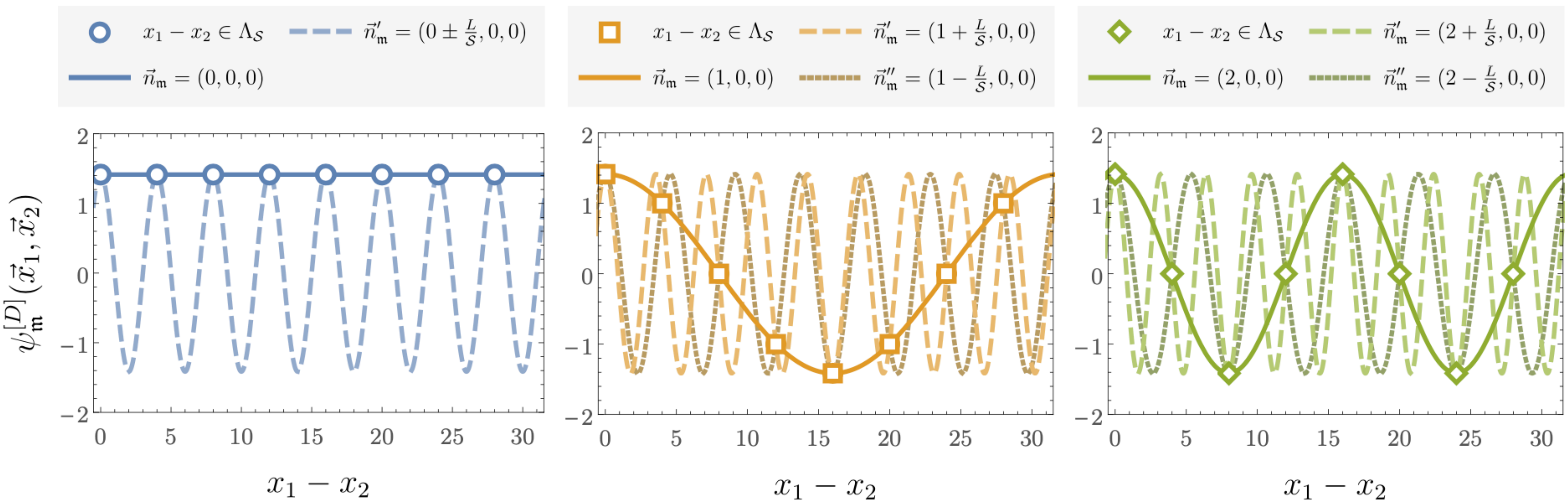
Non-interacting two-baryon FV energy eigenstates involve color singlet baryons

$$D_{\rho\mathfrak{m}s}(t) = \sum \psi^{[D]}_{\mathfrak{m}}(\vec{x}_1, \vec{x}_2) \sum v^{\rho}_{\sigma\sigma'} \frac{1}{\sqrt{2}} \left[p_{\sigma s}(\vec{x}_1, t) n_{\sigma' s}(\vec{x}_2, t) + (-1)^{1-\delta_{\rho 0}} n_{\sigma s}(\vec{x}_1, t) p_{\sigma' s}(\vec{x}_2, t) \right]$$

With plane-wave product wave functions

$$\psi^{[D]}_{\mathfrak{m}}(\vec{x}_1, \vec{x}_2) = e^{i\vec{k}_{\mathfrak{m}} \cdot (\vec{x}_1 - \vec{x}_2)} \qquad \vec{k}_{\mathfrak{m}} = \frac{2\pi \vec{n}_{\mathfrak{m}}}{L}$$

Quark propagator sparsening leads to incomplete Fourier projection and mixing with higher modes, but these are negligible compared to other excited states



Amarasinghe, MW et al, arXiv:2108.10835

Quasi-local operators

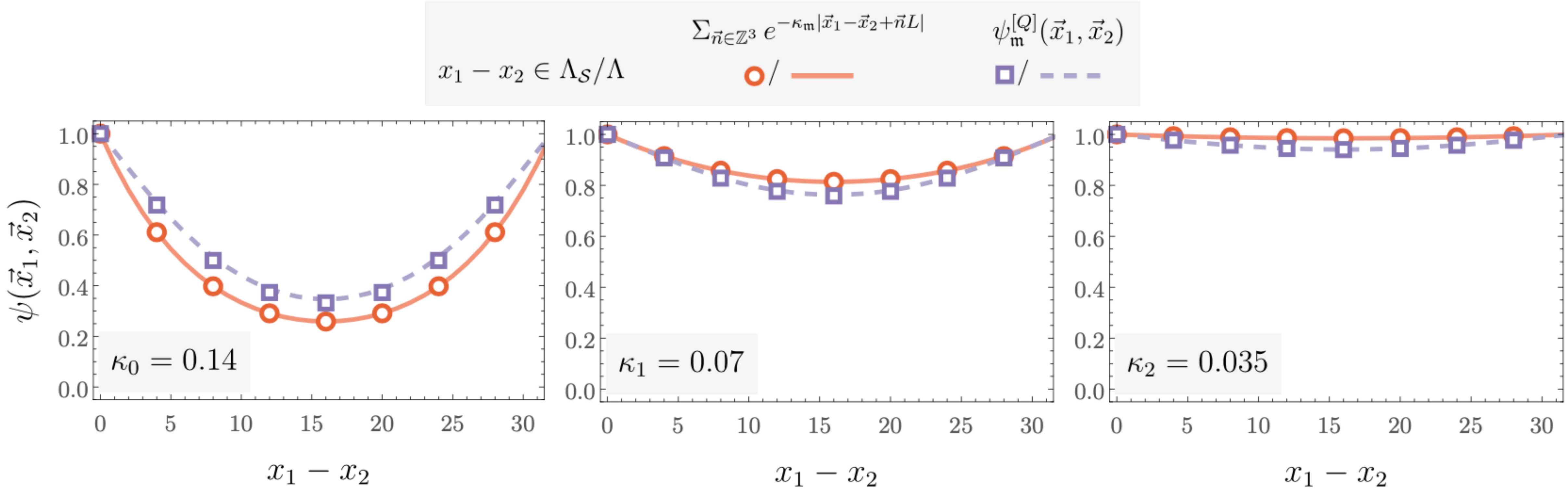
What about loosely bound systems like the deuteron?

Finite-volume EFT wavefunction: $$\sum_{\vec{n}\in\mathbb{Z}_3} e^{-\kappa|\vec{x}_1-\vec{x}_2+n\vec{L}|}\left(\frac{\mathcal{A}}{|\vec{x}_1-\vec{x}_2+\vec{n}L|}+\ldots\right)$$

See e.g. Koning, Lee, and Hammer, Annals Phys. 327, 1450 (2012)
Briceño, Davoudi, Lee and Savage, PRD 88 (2013)

Doesn't factorize into product of single-baryon wavefunctions, no baryon blocks…

Factorizable approximation: $$\psi_{\mathfrak{m}}^{[D]}(\vec{x}_1,\vec{x}_2)=\sum_{\tau\in\mathbb{T}_{\mathcal{S}}} e^{-\kappa_{\mathfrak{m}}|\tau(\vec{x}_1)-\vec{R}|}e^{-\kappa_{\mathfrak{m}}|\tau(\vec{x}_2)-\vec{R}|}$$

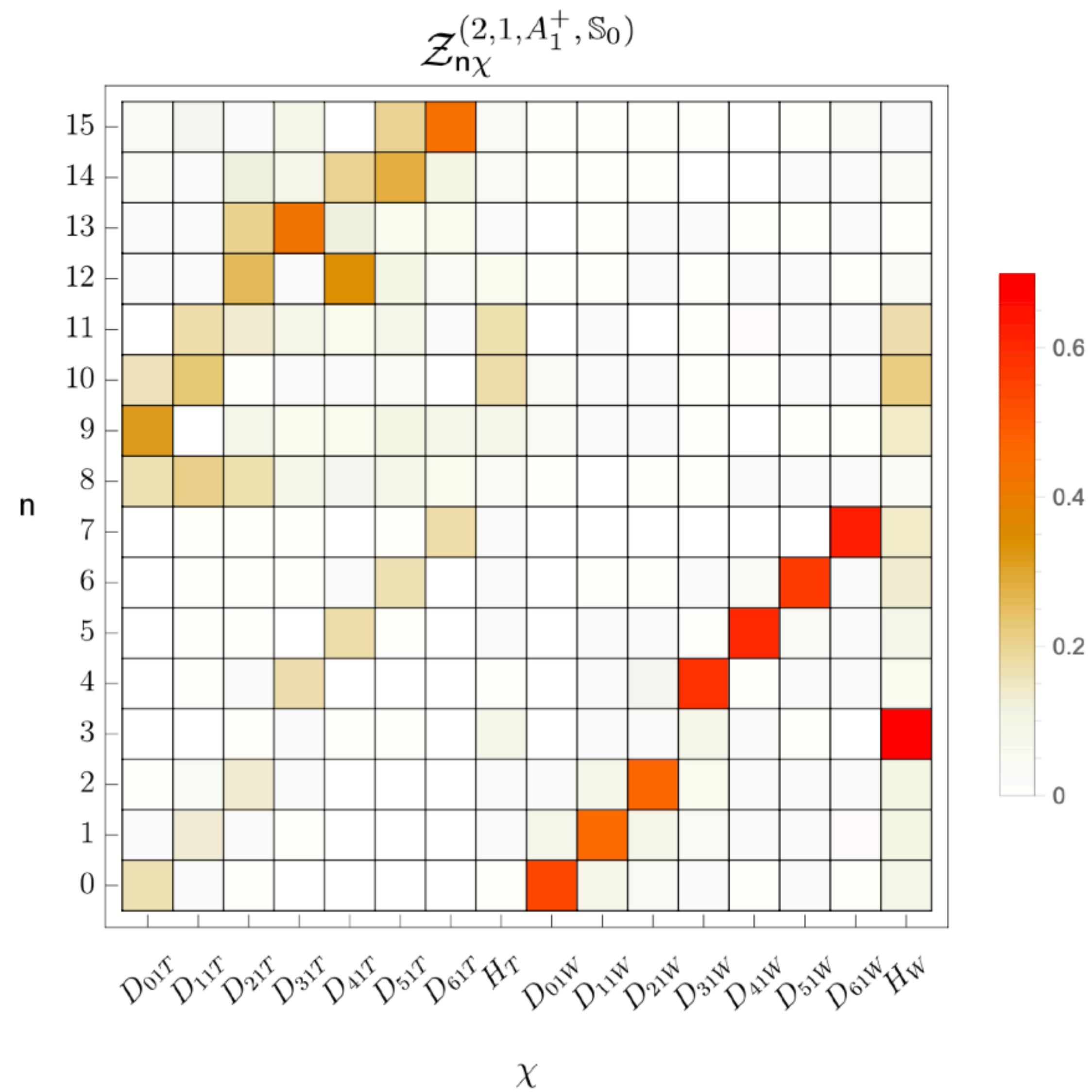


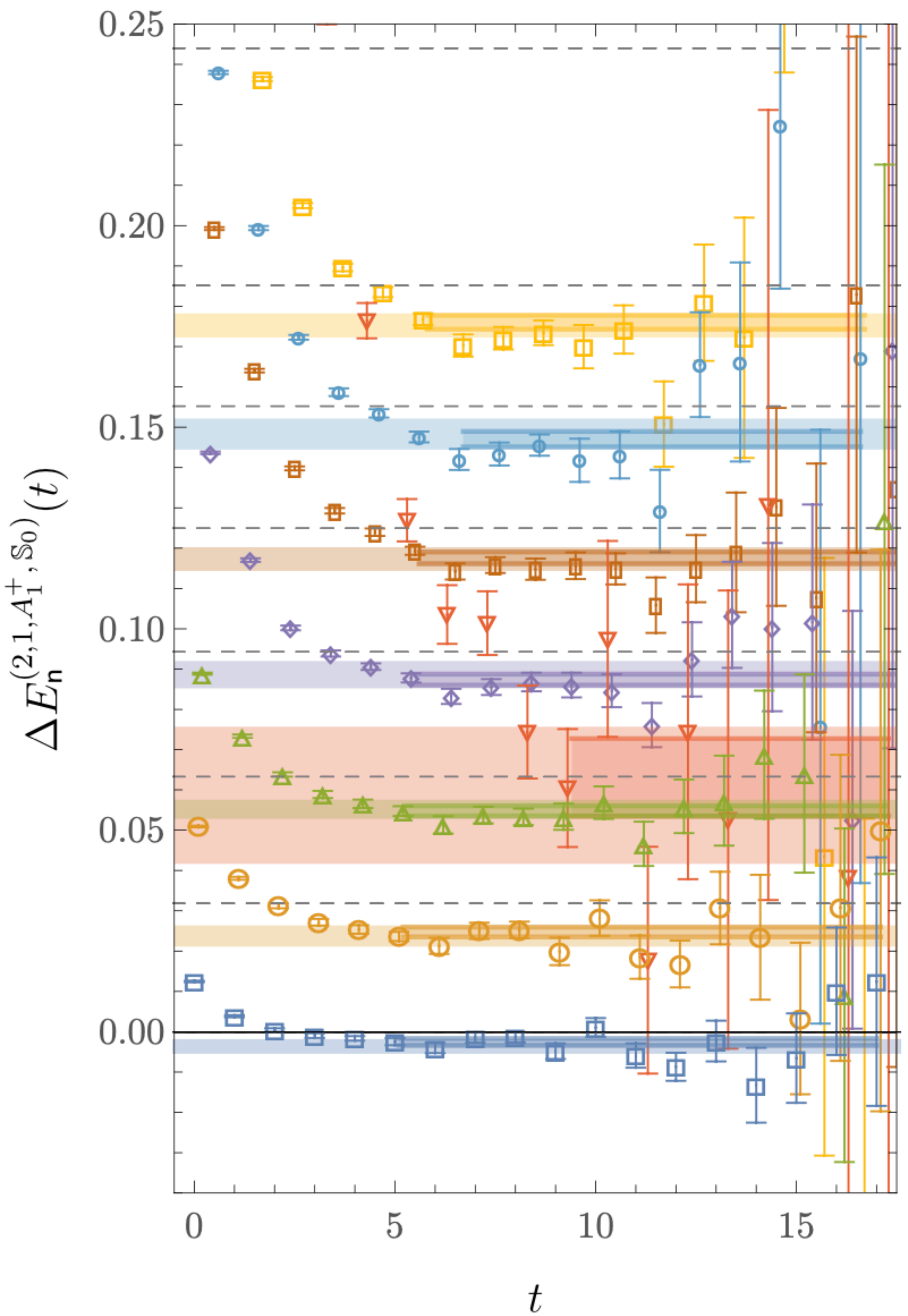
Amarasinghe, MW et al, arXiv:2108.10835

Two nucleons in a box

Diagonalization of correlation-function matrices can be used to remove excited-state contamination from states strongly overlapping with other operators

Each energy level dominantly overlaps with one operator structure, sub-dominant operators collectively 30%





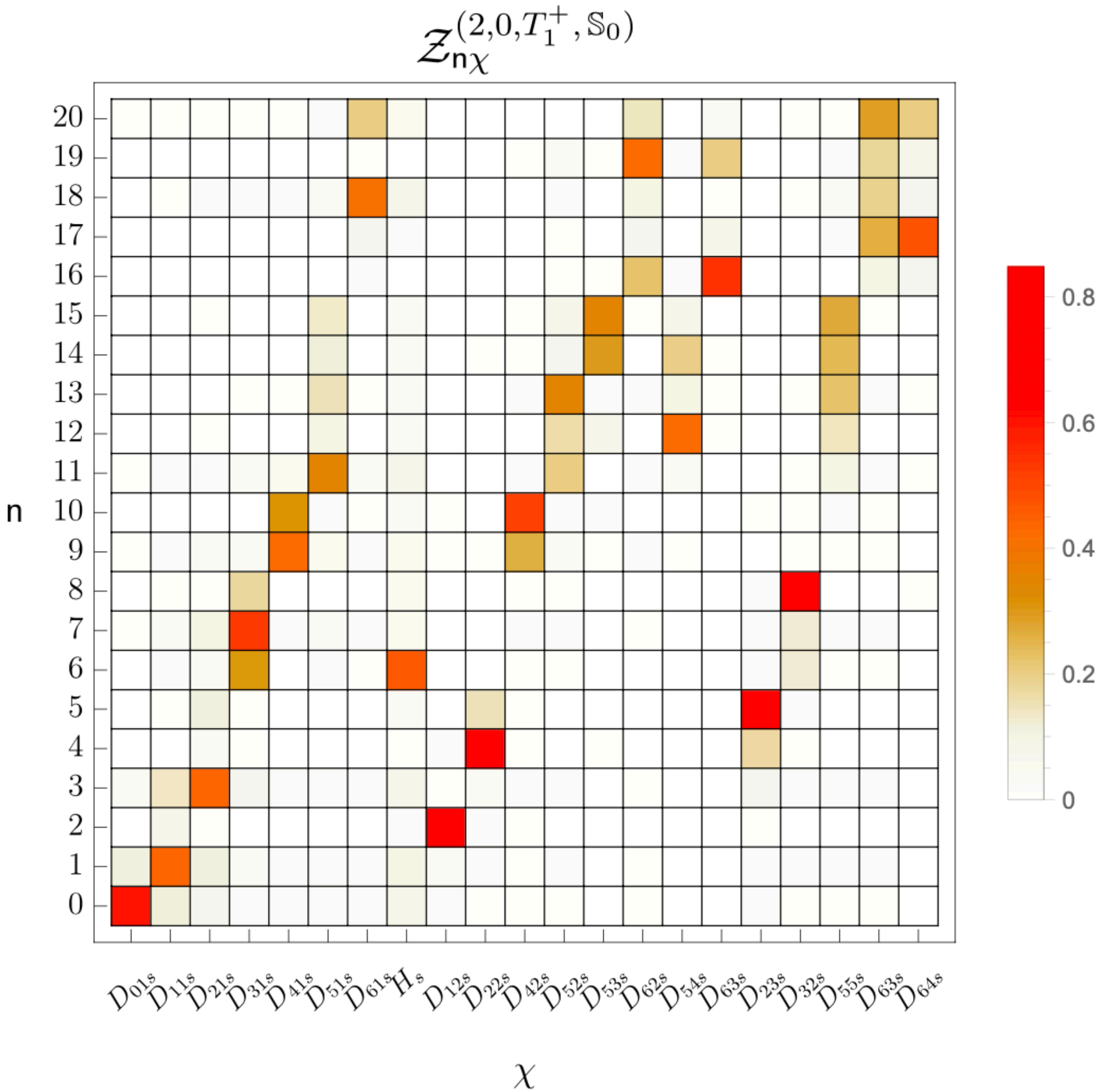
Amarasinghe, MW et al, arXiv:2108.10835

Building a deuteron

Spin-orbit coupling leads to the appearance of many different "orbital angular momentum" wavefunctions transforming in the same cubic group irrep

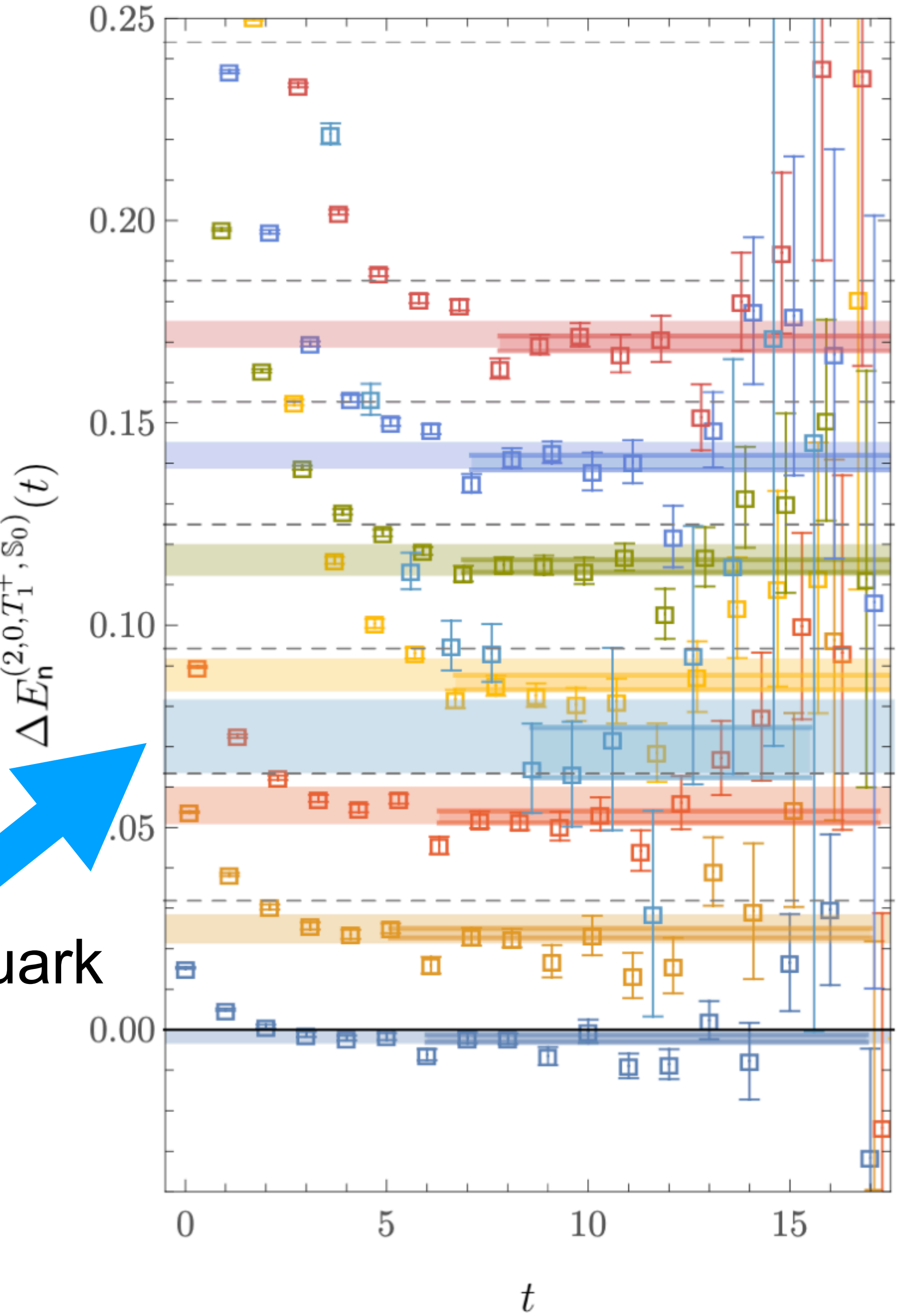
Different dibaryon and hexaquark interpolating operator structures are again approximately orthogonal

Interpolating operator sets including quasi-local alongside dibaryon operators are degenerate in both channels (at current statistical precision)



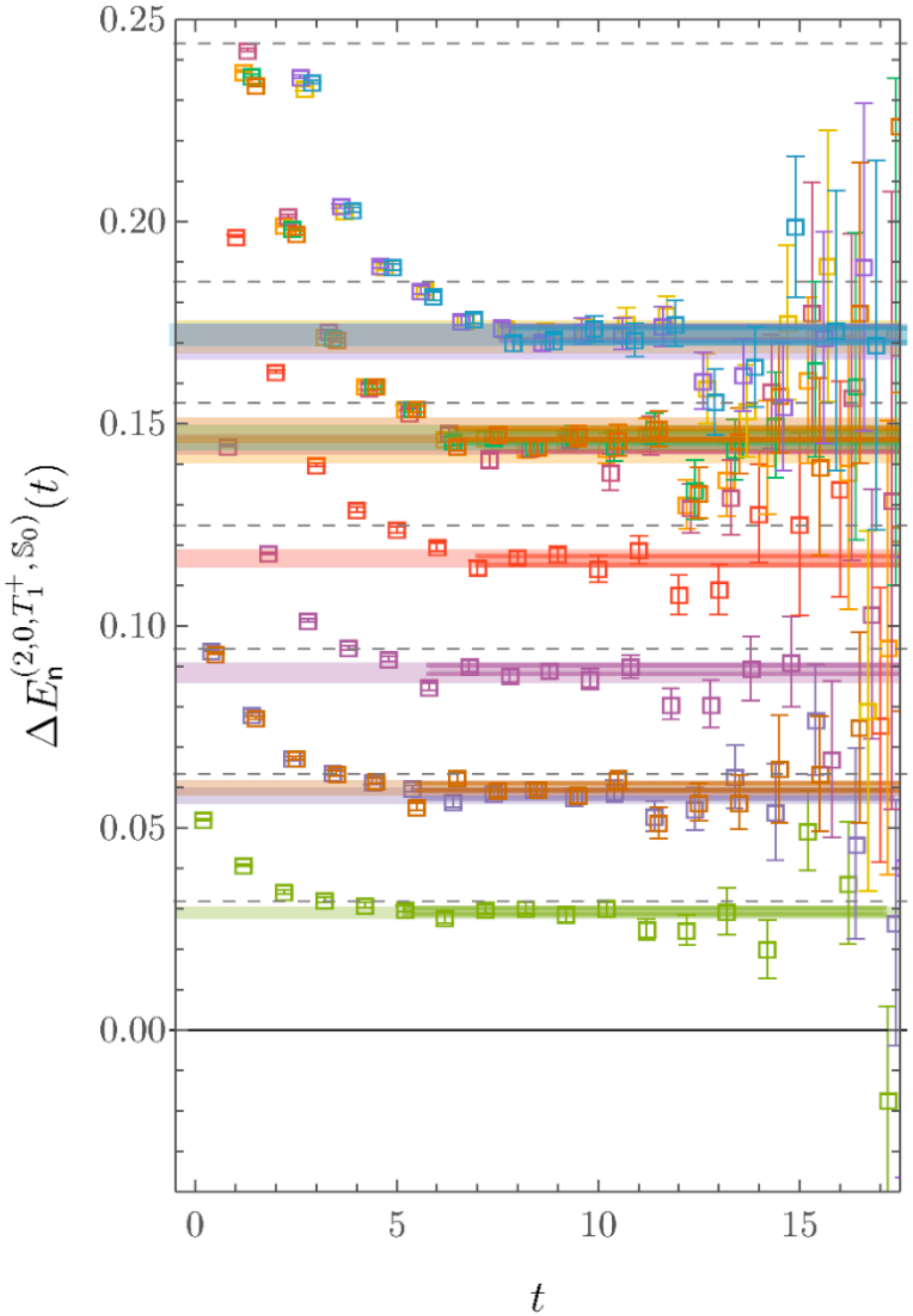
Amarasinghe, MW et al, arXiv:2108.10835

Deuteron variational energy levels



Mostly hexaquark

Cubic analog of *S*-wave



Cubic analog of *D*-wave, *G*-wave, …

Amarasinghe, MW et al, arXiv:2108.10835

Interpolating-operator dependence

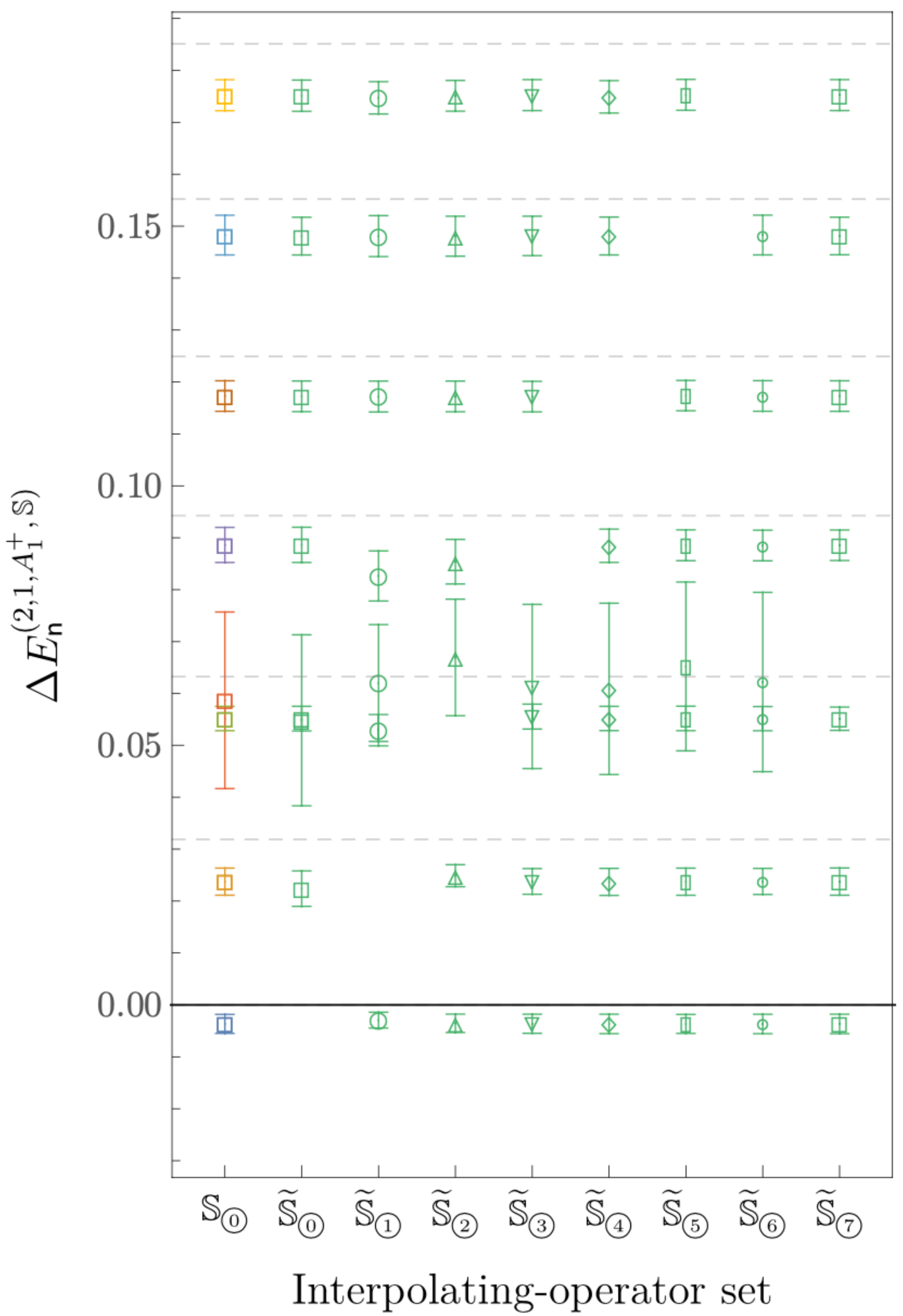
Removing the operator structure with maximum overlap on to a given energy level leads to “missing energy levels”

Even with 10s of interpolating operators, possible to “miss” ground-state

— valid lower bound on ground-state energy, but best-fit results can differ by 5+ σ

Consistent with various dibaryon and hexaquark operators being approximately orthogonal

Much larger ($t \gtrsim 1/\delta \sim 5 \text{ fm}$) source/sink separations would be needed to resolve spectrum using interpolating-operator set missing dominant operators



Amarasinghe, MW et al, arXiv:2108.10835

Missing state toy model

Toy model: 3 state system, 2 interpolating operators

$$Z_{\mathsf{n}}^{(A)} = (\epsilon, \sqrt{1-\epsilon^2}, 0) \qquad Z_{\mathsf{n}}^{(B)} = (\epsilon, 0, \sqrt{1-\epsilon^2})$$

- Both operators have small overlap ϵ with ground state
- Both have ≈ 0 overlap with the state that the other has maximum overlap with

Spectrum

$$E_0^{(AB)} = \eta - \Delta \qquad E_1^{(AB)} = \eta \qquad E_2^{(AB)} = \eta + \delta$$

Correlation-function matrix

$$C^{(AB)}(t) = \sum_{\mathsf{n}} \begin{pmatrix} \left(Z_{\mathsf{n}}^{(A)}\right)^2 & Z_{\mathsf{n}}^{(A)} Z_{\mathsf{n}}^{(B)} \\ Z_{\mathsf{n}}^{(A)} Z_{\mathsf{n}}^{(B)} & \left(Z_{\mathsf{n}}^{(B)}\right)^2 \end{pmatrix} e^{-E_{\mathsf{n}}^{(AB)} t}$$

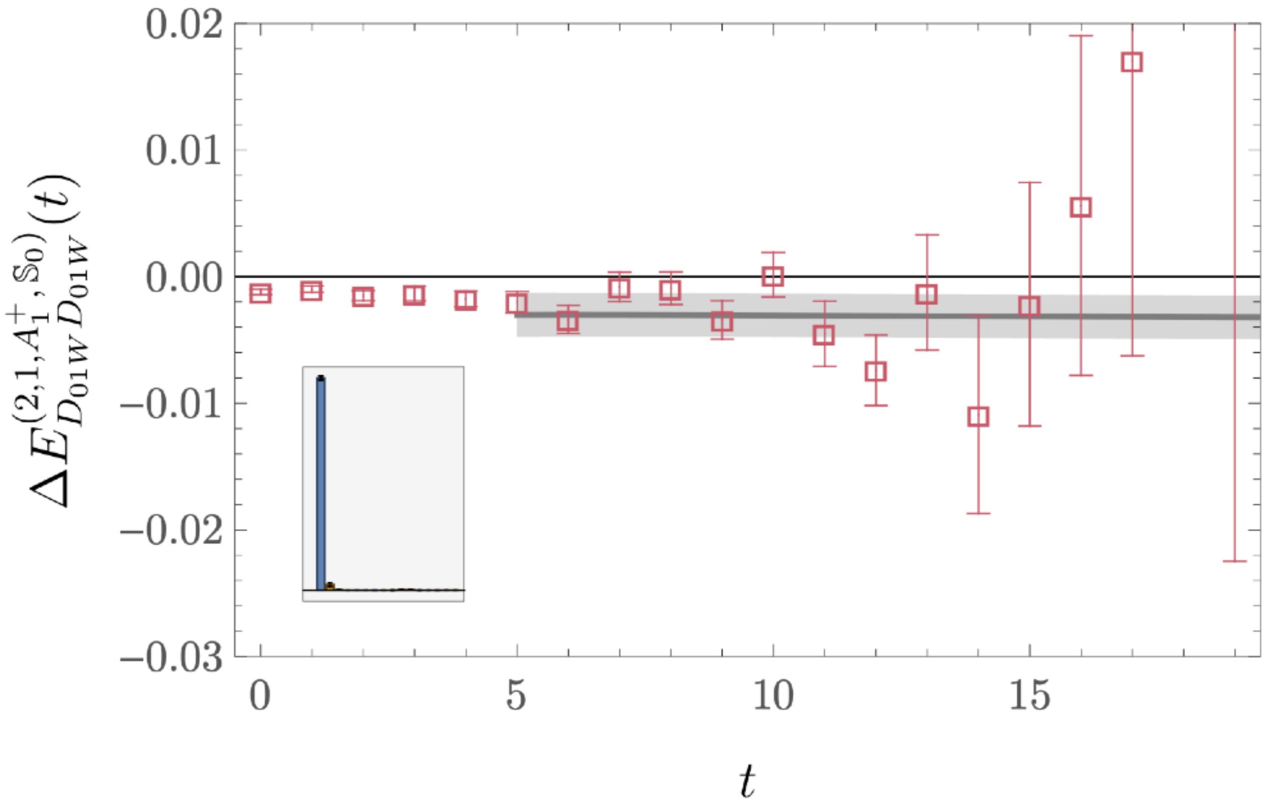
Eigenvalues:

$$\lambda_0^{(AB)} = e^{-(t-t_0)\eta} \left[1 + \epsilon^2 (e^{t\Delta} - e^{t_0 \Delta}) + \mathcal{O}(\epsilon^4)\right]$$

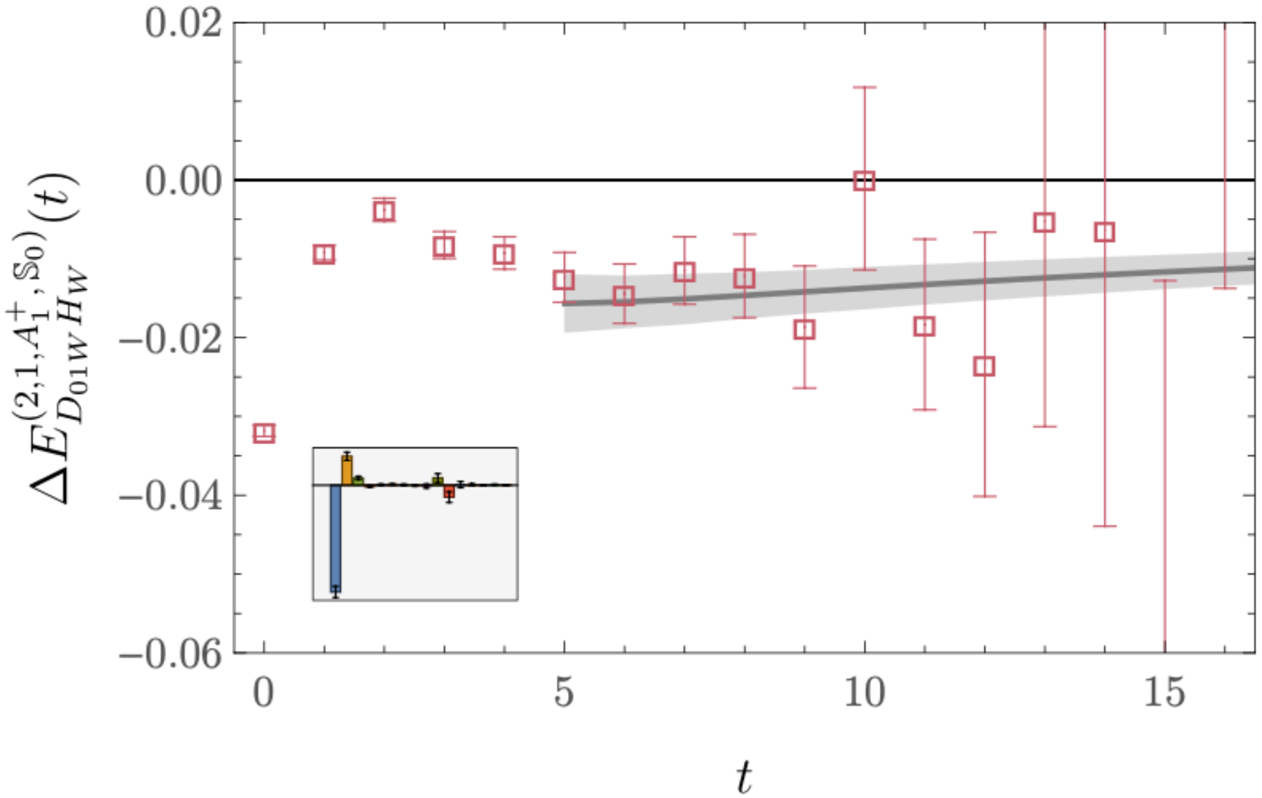
$$\lambda_1^{(AB)} = e^{-(t-t_0)(\eta+\delta)} \left[1 + \epsilon^2 (e^{t(\Delta+\delta)} - e^{t_0(\Delta+\delta)}) + \mathcal{O}(\epsilon^4)\right]$$

Variational predictions

Dibaryon-dibaryon, [*D*, *D*], correlation functions ~ 95% ground-state contribution in reconstruction using same operator set



Reconstructions of [*D*, *H*] correlation functions using spectrum from variational methods can reproduce LQCD results

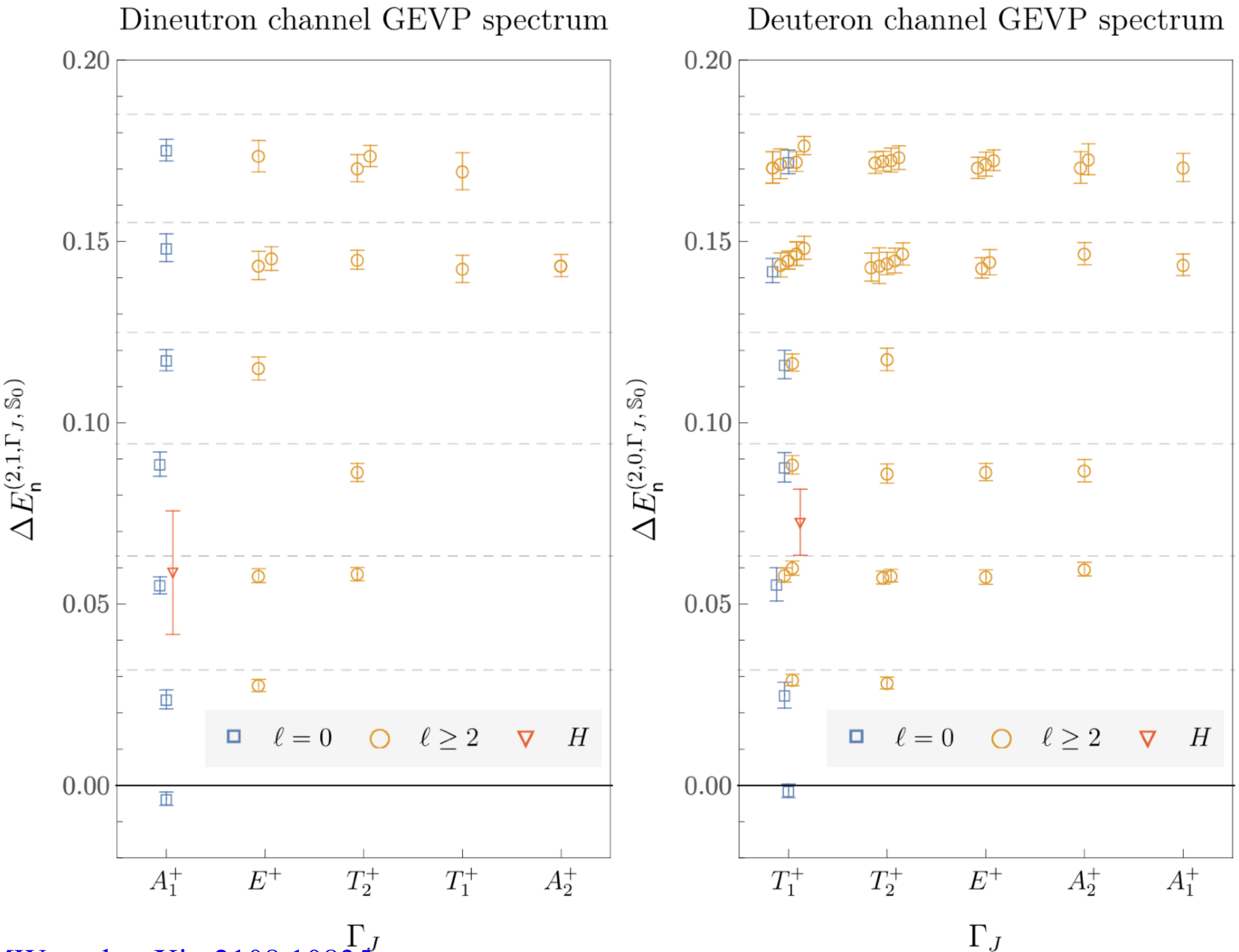


Variational method results provide model of spectrum in which [*D*, *H*] correlation functions approach ground-state from below

Amarasinghe, MW et al, arXiv:2108.10835

Variational energy spectrum

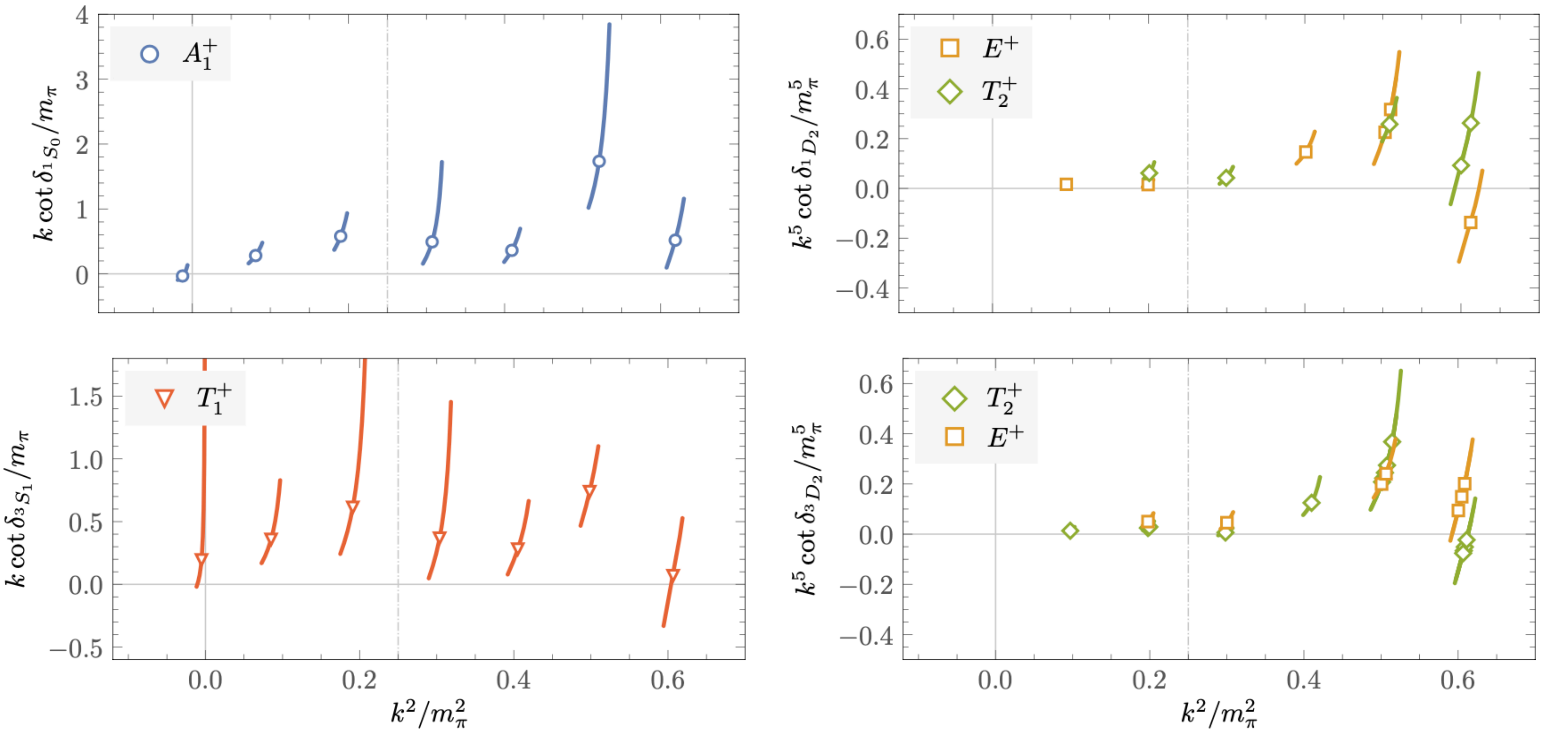
For a given interpolating-operator set, two-nucleon finite-volume energy spectrum can be extracted in various cubic irreps associated with *S*-wave, *D*-wave, and higher-partial-wave interactions



Amarasinghe, MW et al, arXiv:2108.10835

Variational phase shift results

Finite-volume spectrum can be mapped to *S*-wave, *P*-wave and higher-partial-wave scattering phase shifts using generalizations of Lüscher's quantization condition



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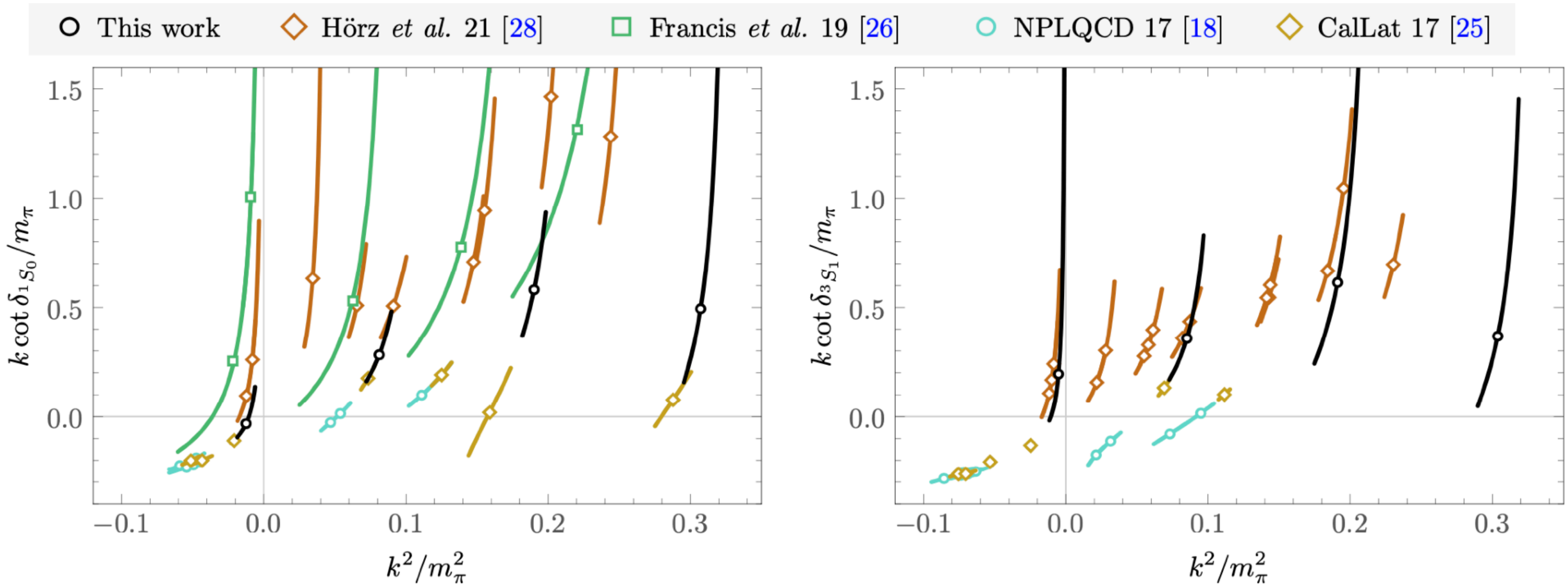
NN phase shift comparisons



S-wave phase shift results using variational methods and symmetric dibaryon correlation functions consistent among several groups

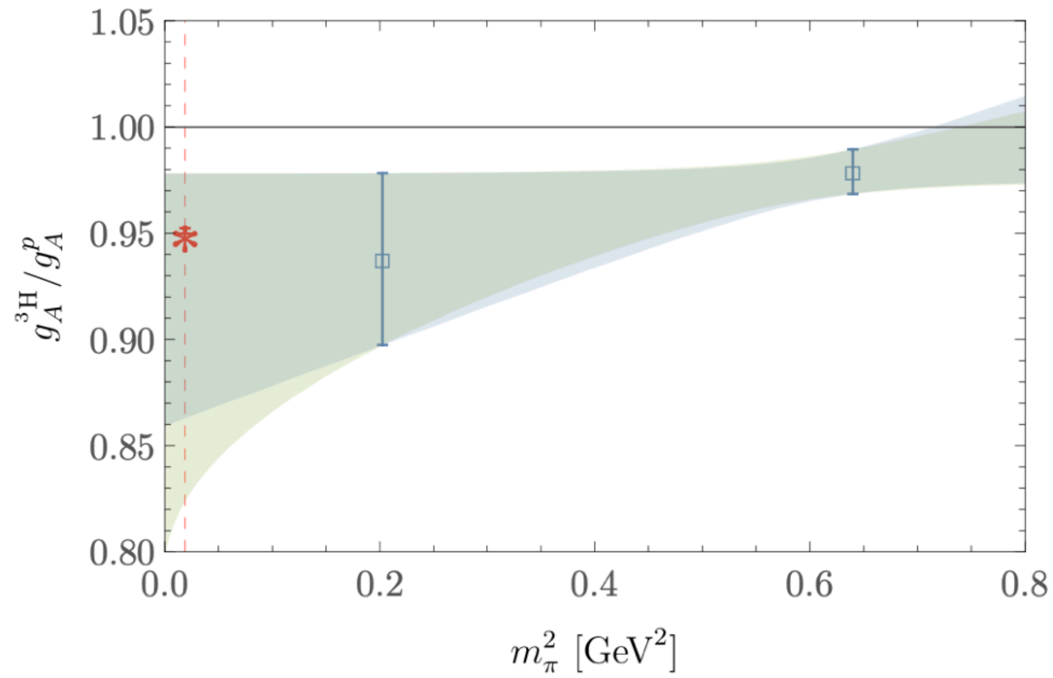
Discrepancies with previous results using dibaryon-hexaquark correlation functions on the same gauge-field ensemble from multiple groups

Further variational studies are needed to conclusively determine whether two-nucleon systems bind with heavier-than-physical quark masses

Amarasinghe, MW et al, arXiv:2108.10835

Outlook

LQCD calculations of nuclear matrix elements can constrain EFTs and nuclear models relevant for neutrino-nucleus scattering, double-beta decay, and other new physics searches



Low-energy excited states lead to significant and hard-to-quantify systematic uncertainties in multi-nucleon correlation functions

Future variational studies exploring the Hilbert space possibly associated with a bound state are required to conclusively determine with two-nucleon systems bind with heavier than physical quark masses