Towards Lattice QCD Calculations of Pion Production

Fermilab

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Motivation

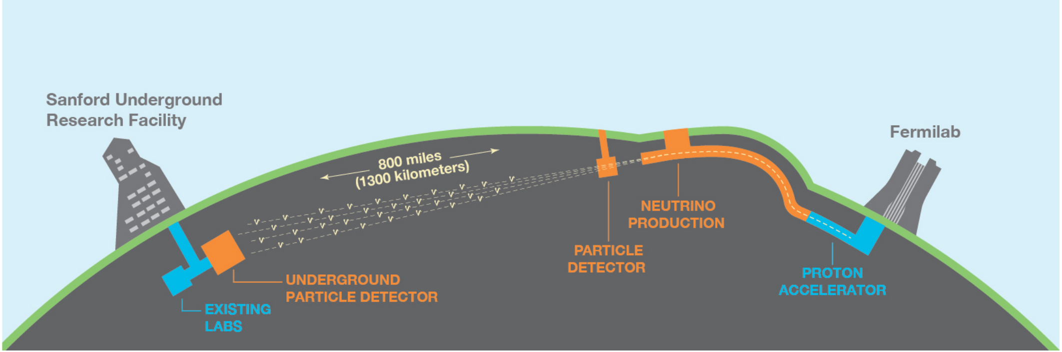


Image credit: Fermilab

Deep Underground Neutrino Experiment

- Beam from Fermilab to South Dakota to study ν oscillations
- Oscillation parameters depend on $P(\nu_\mu \to \nu_e)$ as function of L/E
- Experimental ν beams inherently broadband
- Will require reconstruction of E_ν
- Need energy-dependent cross-sections for ν-nucleus interactions

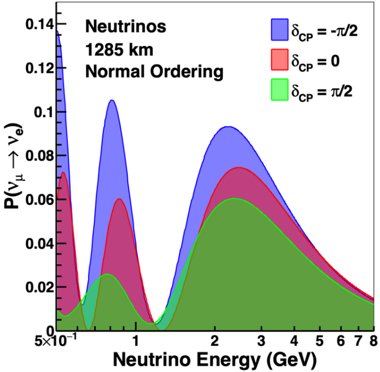
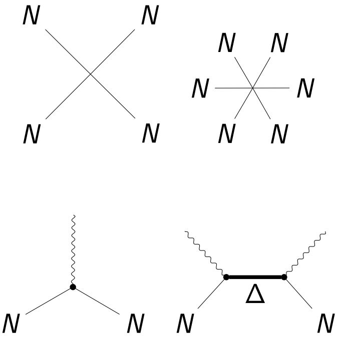


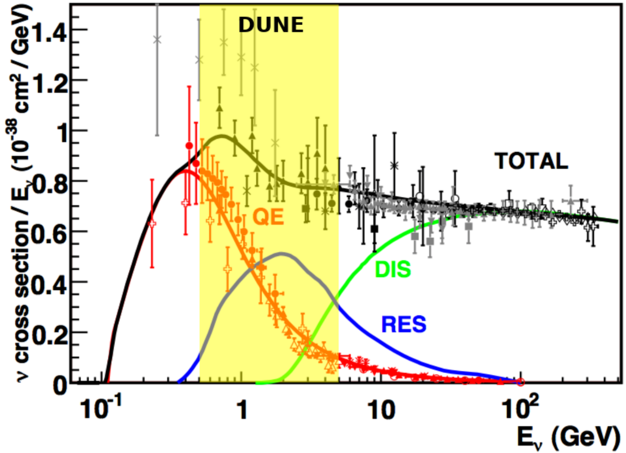
Image credit: B. Abi et al. (DUNE Collaboration), 2006.16043

ν-A Cross-Sections

- Several varieties of nuclear many-body methods (A. Lovato, Tues. 9:00)
  - GFMC (J. Carlson et al., 1412.3081), AFDMC (A. Lovato et al., 2206.10021), spectral functions (N. Steinburg, Tues. 11:10)
- All require nuclear Hamiltonian + couplings to external currents
- ν-A cross-sections $\leftarrow$ ν-N cross-sections



ν-N Cross-Sections



- Quasi-elastic regime – based on nucleon elastic form factor
- DIS regime – perturbative
  - Factorization theorems, nucleon PDFs
- Resonant regime – dominated by $N \to \Delta$
  - Peak of DUNE beam
  - Need $\sim$3% uncertainty for DUNE (D. Simons et al., 2210.02455)

Image credit: Adapted from J. A. Formaggio, G. P. Zeller (1305.7513)

Δ Neutrinoproduction

$$\nu_\mu N \to \mu\Delta$$

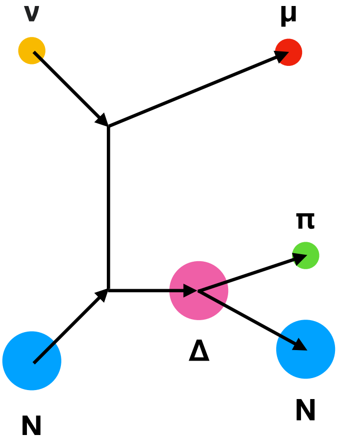
- Mediated through electroweak current

$$\bar{N}(\gamma_\mu - \gamma_\mu\gamma_5)\Delta$$

- Vector component known from $eN \to e\Delta$
- Axial component difficult to measure experimentally
- Δ resonance above $N\pi\pi$ threshold

$$\Delta \to N\pi, N\pi\pi$$

- Goal: Understand $N\pi$, $N\pi\pi$ spectrum up to m_Δ



$N \to \Delta$ Form Factors

- $N \to \Delta$ transition factorizes as

$$\langle \Delta(p', s') | A^3_\mu | N(p, s) \rangle = i\sqrt{\frac{2}{3}} \left(\frac{m_\Delta m_N}{E_\Delta(\mathbf{p}') E_N(\mathbf{p})} \right)^{1/2}$$
$$\bar{u}^\lambda_\Delta \left[\left(\frac{C^A_3(q^2)}{m_N} \gamma^\nu + \frac{C^A_4(q^2)}{m_N^2} p'^\nu \right) \left(g_{\lambda\mu} g_{\rho\nu} - g_{\lambda\rho} g_{\mu\nu} \right) q^\rho + C^A_5(q^2) g_{\lambda\mu} + \frac{C^A_6(q^2)}{m_N^2} q_\lambda q_\mu \right] u_N$$

- Need to extract C^A_3, C^A_4, C^A_5, C^A_6 as functions of q^2

Bubble Chamber Fits

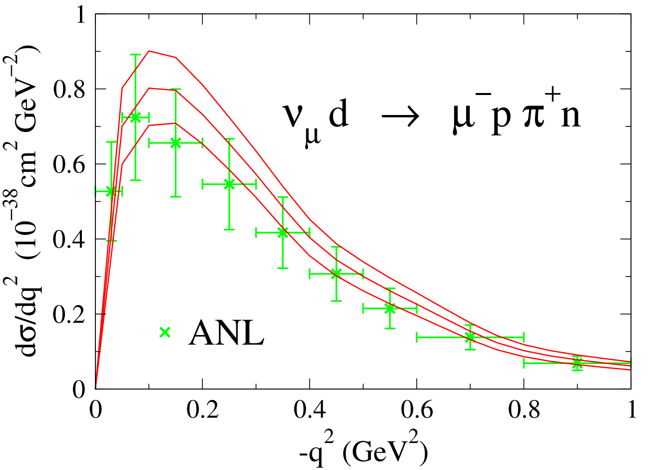
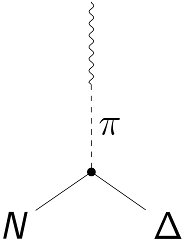


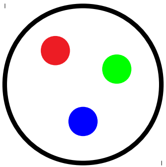
Figure credit: E. Hernandez et al., 1001.4416

Extracting Form Factors

- Target: Know all $C_i^A(q^2)$ with few-percent uncertainty
- Experimental data have large ($\gtrsim 15\%$) statistical uncertainties
- Additional systematic uncertainties from deuteron binding
- 4 form factors – need to measure various kinematics, polarizations
- Models of QCD $\rightarrow$ relations among C_i^A
- Uncontrolled systematics from model assumptions



$$C_5^A \propto Q^2 C_6^A$$



$$C_3^A \sim 0$$

$$C_4^A \sim -\frac{C_5^A}{4}$$

Lattice QCD

- Discretize equations of QCD on 4-dimensional space-time lattice
- Finite box required (extrapolate $L \to \infty$ at end)
- Non-perturbative (works for large coupling constants)
- First-principles, model-independent solution to hadronic physics
- Only input = Lagrangian of QCD ($\{m_q\}, \alpha_s$)
- Systematically controllable errors (A. Kronfeld, Mon. 1:30 pm)

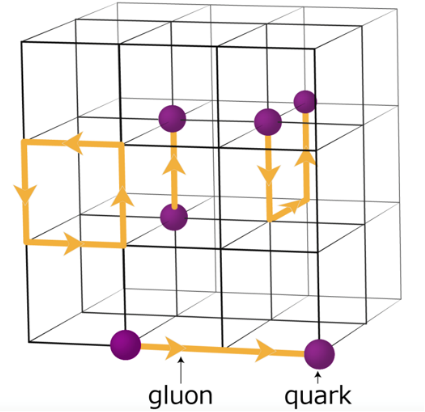


Image credit: JICFuS, Tsukuba

Brute Force Is The Last Resort of the Incompetent

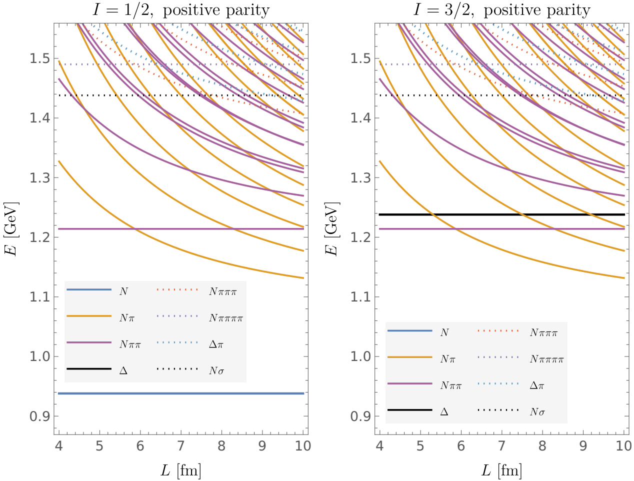
Image credit: Oak Ridge National Laboratory

Finite Volume Spectrum

$$E_{N\pi} = \sqrt{m_N^2 + \mathbf{p}^2} + \sqrt{m_\pi^2 + \mathbf{p}^2}$$

$$\mathbf{p} \in 2\pi\mathbb{Z}^3/L$$

- Parities: $P(N) = P(\Delta) = 1$, $P(\pi) = -1$
- $P(N\pi) = -1$, needs momentum to match $P(\Delta)$
- $P(N\pi\pi) = 1 = P(\Delta)$ even at $\mathbf{p} = 0$



Matching to Many-Body

Two main options to match to nuclear EFT:

1. Lellouch-Lüscher formalism (Lellouch and Lüscher, hep-lat/0003023; Briceño et al., 1706.06223)
   - Extrapolate lattice results to infinite volume
   - Relies on extracting phase shifts from FV spectrum
   - Worked out in 2-particle case, progress in 3-particle case but not completely resolved (Hansen and Sharpe, 1901.00483)
2. Finite-volume EFT matching
   - Perform nuclear EFT calculations within finite box
   - Can then match directly to lattice QCD calculation

Excited State Contamination

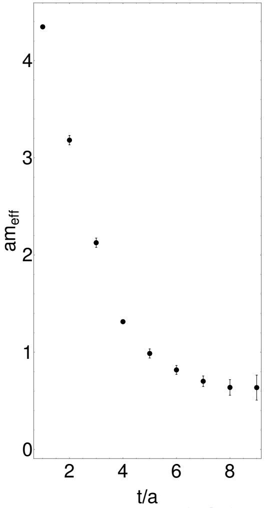
- Determine particle energies from correlation functions

$$C_2(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0)\rangle = \sum_n \frac{Z_n^2}{2E_n} e^{-E_n t}$$

  - Sum runs over all states with same quantum numbers as $\mathcal{O}$
- At large Euclidean time, dominated by ground state

$$C_2(t) \to \frac{Z_0^2}{2E_0} e^{-E_0 t}$$

- Cannot take $t \to \infty$ due to noisy data
- At moderate t, can have contamination from higher-energy states



Importance of $N\pi$ State

- Need to compute $N \rightarrow N$ matrix elements for form factors
- $N\pi$ only separated from N by m_π (if $L = \infty$)
- $N\pi$ final state suppressed by $e^{-m_\pi t}$
  - $e^{-m_\pi t} \approx 0.25$ if $t = 2$ fm
  - Overlap factors Z_n can be large for $N\pi$ states
- Form factors can be wrong due to contamination unless $N\pi$ state accounted for (R. Gupta, Mon. 2:40 pm)

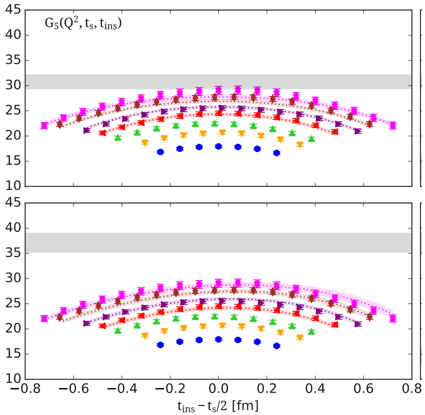


Figure credit: C. Alexandrou et al., 2011.13342

Variational Methods

- Interpolating operator $\mathcal{O}$ for state not unique
- Can take many operators $\{\mathcal{O}_i\}$ with same quantum numbers
- $\mathcal{O}_i$ will have different overlaps to ground, excited states $\rightarrow$ different contamination
- Optimal linear combination of $\mathcal{O}_i$ has minimal contamination
  - Found via generalized eigenvalue problem (GEVP)

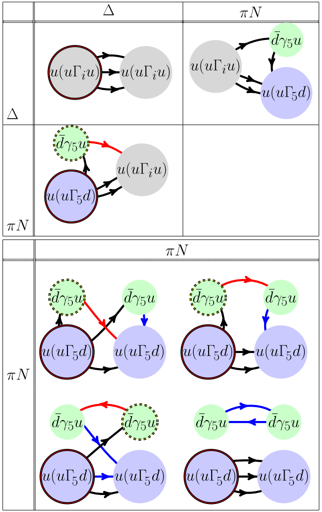


Figure credit: G. Silvi et al., 2101.00689

Δ Resonance on Lattice

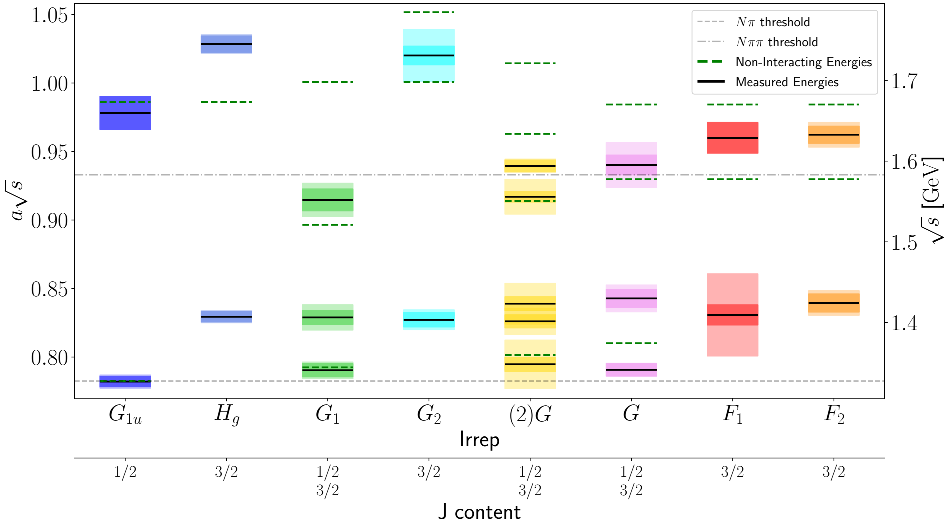


Figure credit: G. Silvi et al., 2101.00689

Importance of $N\pi\pi$ State

- Useful to remove states above energy level of interest
- Essential to understand those below level of interest
- $m_N + 2m_\pi < m_\Delta$ (1.21 GeV < 1.23 GeV)

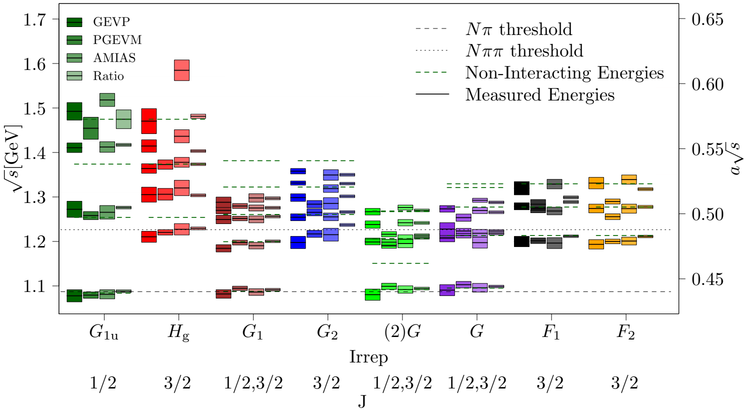


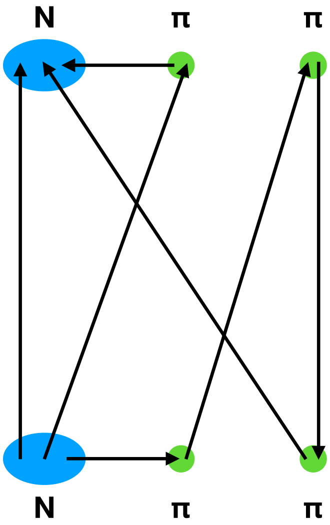
Figure credit: C. Alexandrou et al., 2307.12846

Methodology

- Want to compute

$$\langle N(\tau)\pi(\tau)\pi(\tau)\bar{N}(0)\bar{\pi}(0)\bar{\pi}(0)\rangle$$

- Naïvely requires all-to-all propagators (timeslice-to-self π loops)
- Cost: $O(V^2)$ for inversions, $O(V^6)$ for contractions
- Contraction cost reduced to $O(V^3)$ by computing sequential propagators through π
- Contraction cost further reduced by eightfold by parity projecting all quarks



Propagator Sparsening

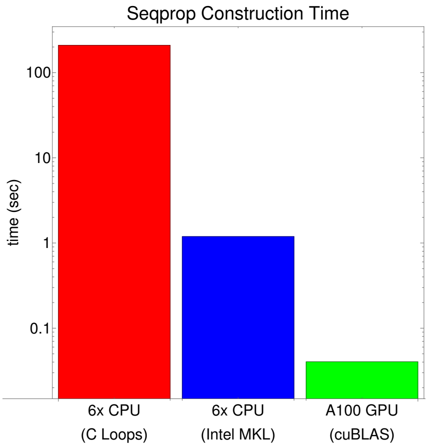
- Nearby sites on lattices highly correlated
- Can compute propagators on coarse grid without much loss of information (W. Detmold et al., 1908.07050; Y. Li, 2009.01029; S. Amarasinghe et al., 2108.10835)
    - In momentum space, corresponds to incomplete Fourier projection
- Loss of information further reduced by Gaussian smearing
- Sparsening by factor of f in each direction reduces inversion costs by f^3 and seqprop construction cost in contractions by f^9

Ensemble Details

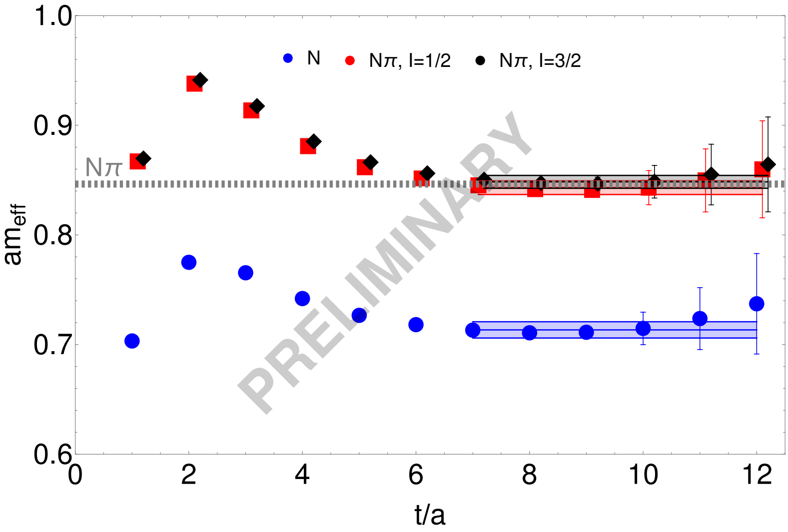
- $a = 0.15$ fm, $L = 4.8$ fm, $m_{\pi,P} = 135$ MeV HISQ ensemble from FNAL/MILC
- Clover fermions used for valence quarks ($m_{\pi,\mathrm{val}} \approx 170$ MeV)
- Gradient flow smearing used to reduce mixed-action artifacts
- Propagators computed using QUDA multigrid inverter (M. Clark et al., 0911.3191, 1612.07873) on 8^3 grid on each timeslice
- Gaussian smearing applied at source and sink

Contraction Code

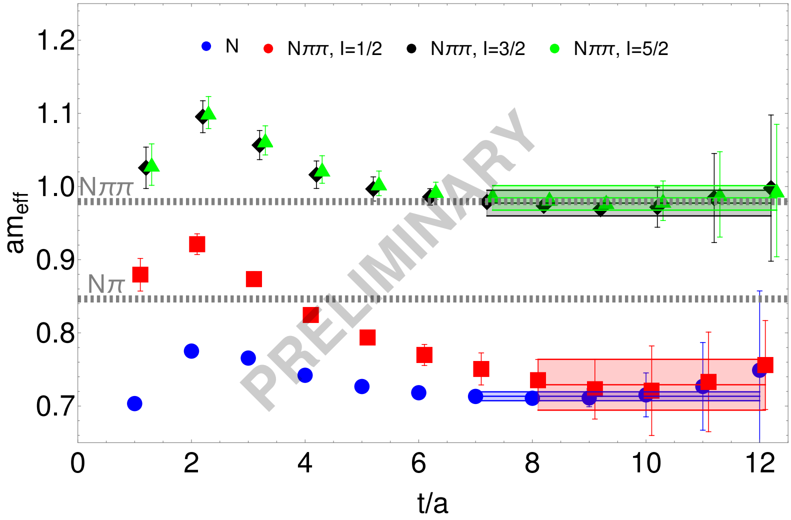
- Standalone code to read in propagators from QUDA and compute $N\pi$, $N\pi\pi$ contractions
- Designed to support CPU and GPU targets
- Leverages MKL BLAS or cuBLAS for sequential propagator construction
- Performs all Wick contractions from these sequential propagators



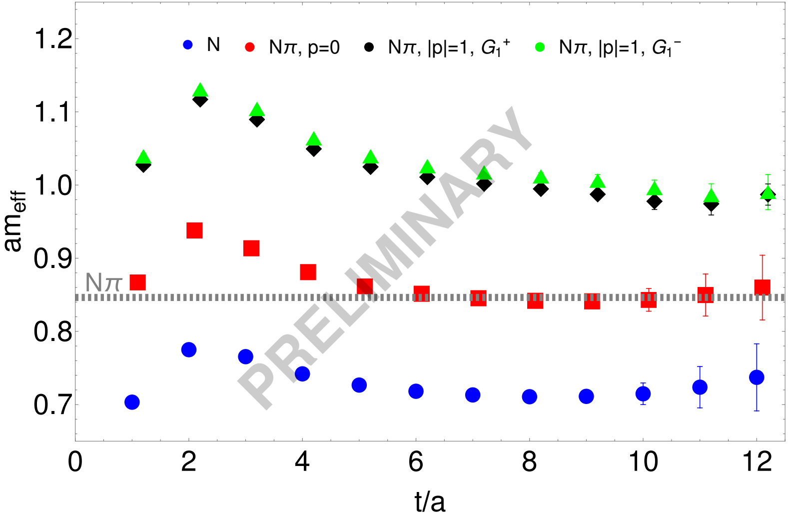
$N\pi$, $\mathbf{p} = 0$



$N\pi\pi$, $\mathbf{p} = 0$



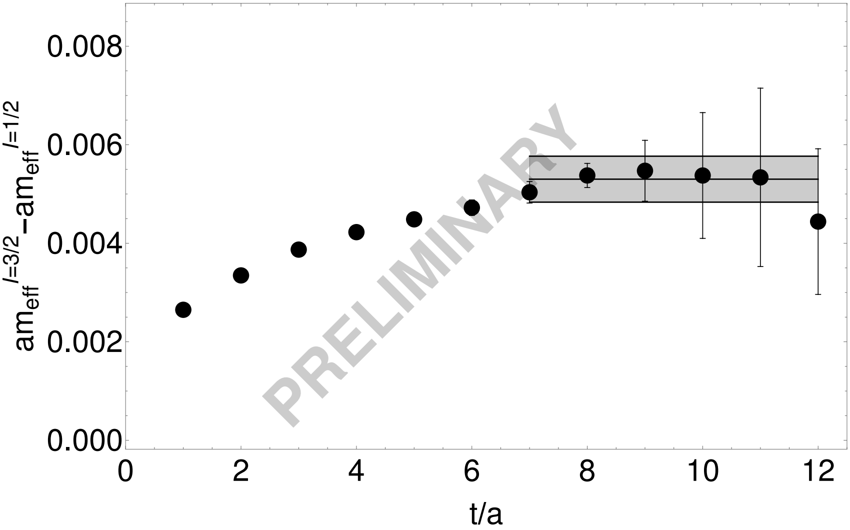
$N\pi,\ I = 1/2,\ |\mathbf{p}| = 1$



Conclusions

- $N \to \Delta$ and therefore $N \to N\pi, N\pi\pi$ axial transitions needed for DUNE
- Spectroscopy calculations – first step in producing good $N\pi(\pi)$ interpolators
- Future plans:
  - Increased statistics
  - GEVP to study states in same parity/isospin sectors
  - Finite-volume phase shifts to study Δ resonance
  - 3-point functions for axial/vector form factors

Isospin Splitting in $N\pi$



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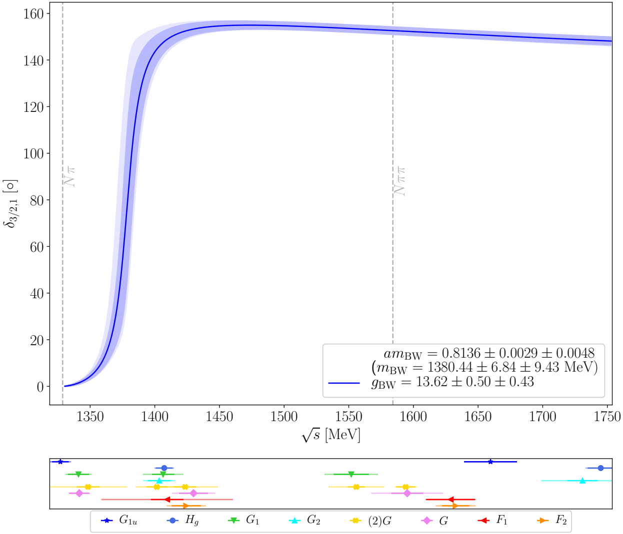

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